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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JUL 20	Powerful new interactive analysis and visualization software, STN AnaVist, now available
NEWS	4	AUG 11	Derwent World Patents Index(R) web-based training during August
NEWS	5	AUG 11	STN AnaVist workshops to be held in North America
NEWS	6	AUG 30	CA/CAplus -Increased access to 19th century research documents
NEWS	7	AUG 30	CASREACT - Enhanced with displayable reaction conditions
NEWS	8	SEP 09	ACD predicted properties enhanced in REGISTRY/ZREGISTRY

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:48:55 ON 21 SEP 2005

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:49:02 ON 21 SEP 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 SEP 2005 HIGHEST RN 863546-28-5
DICTIONARY FILE UPDATES: 20 SEP 2005 HIGHEST RN 863546-28-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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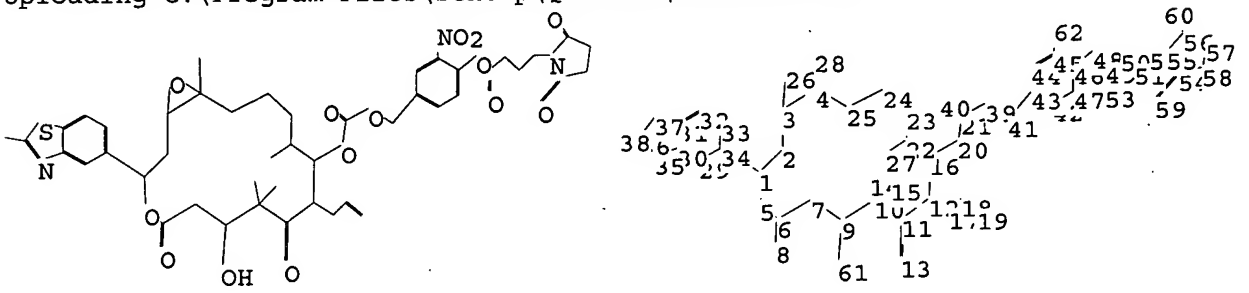
Uploading C:\Program Files\Stnexp\Queries\10631011.str



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8 13 14 15 17 18 19 20 21 27 28 38 39 40 41 48 49 50 51 52 53 59 60 61 62
ring nodes :
1 2 3 4 5 6 7 9 10 11 12 16 22 23 24 25 26 29 30 31 32 33 34 35 36 37 42 43 44 45 46 47 54 55 56 57 58
chain bonds :
1-34 4-28 6-8 9-61 10-14 10-15 11-13 12-17 16-20 17-18 18-19 20-21 21-39 21-40 22-27 36-38 39-41 41-43 45-62 46-48 48-49 49-50 49-53 50-51 51-52 52-55 54-59 56-60

```
ring bonds :
1-2  1-5  2-3  3-4  3-26  4-25  4-26  5-6  6-7  7-9  9-10  10-11  11-12  12-16
16-22  22-23  23-24  24-25  29-30  29-34  30-31  30-35  31-32  31-37  32-33  33-34
35-36  36-37  42-43  42-47  43-44  44-45  45-46  46-47  54-55  54-58  55-56  56-57
57-58
exact/norm bonds :
6-8  9-61  11-13  16-20  20-21  21-39  21-40  30-35  35-36  39-41  46-48  48-49
49-53  52-55  54-55  54-59  55-56  56-60
exact bonds :
1-2  1-5  1-34  2-3  3-4  3-26  4-25  4-26  4-28  5-6  6-7  7-9  9-10  10-11  10-14
 10-15  11-12  12-16  12-17  16-22  17-18  18-19  22-23  22-27  23-24  24-25  31-37
 36-37  36-38  41-43  45-62  49-50  50-51  51-52  54-58  56-57  57-58
normalized bonds :
29-30  29-34  30-31  31-32  32-33  33-34  42-43  42-47  43-44  44-45  45-46  46-47
isolated ring systems :
containing 1 : 29 : 42 : 54 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:CLASS  9:Atom  10:Atom
11:Atom  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:Atom  17:CLASS  18:CLASS
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L1      STRUCTURE UPLOADED

=> s l1
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SAMPLE SCREEN SEARCH COMPLETED -        1 TO ITERATE

100.0% PROCESSED        1 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            1 TO       80
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 17:49:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

L3            1 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             161.76     161.97
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FILE 'CAPLUS' ENTERED AT 17:50:09 ON 21 SEP 2005

FILE COVERS 1907 - 21 Sep 2005 VOL 143 ISS 13
FILE LAST UPDATED: 20 Sep 2005 (20050920/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d l4 ibib hitstr abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:120722 CAPLUS
DOCUMENT NUMBER: 140:181251
TITLE: Preparation of new epothilone peptide effector conjugates for pharmaceutical use in the treatment of proliferative or angiogenesis associated disease processes
INVENTOR(S): Berger, Markus; Siemeister, Gerhard; Klar, Ulrich; Willuda, Joerg; Menrad, Andreas; Bosslet, Klaus
PATENT ASSIGNEE(S): Schering AG, Germany
SOURCE: PCT Int. Appl., 148 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004012735	A2	20040212	WO 2003-EP8483	20030731
WO 2004012735	A3	20040527		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,

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            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     DE 10234975          A1     20040212    DE 2002-10234975       20020731
     DE 10305098          A1     20040819    DE 2003-10305098       20030207
     CA 2492437           AA     20040212    CA 2003-2492437        20030731
     EP 1524979           A2     20050427    EP 2003-743752         20030731
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003013043        A      20050614    BR 2003-13043          20030731
PRIORITY APPLN. INFO.:                       DE 2002-10234975    A  20020731
                                             DE 2003-10305098    A  20030207
                                             US 2003-451673P     P  20030305
                                             WO 2003-EP8483      W  20030731
OTHER SOURCE(S):         MARPAT 140:181251
```

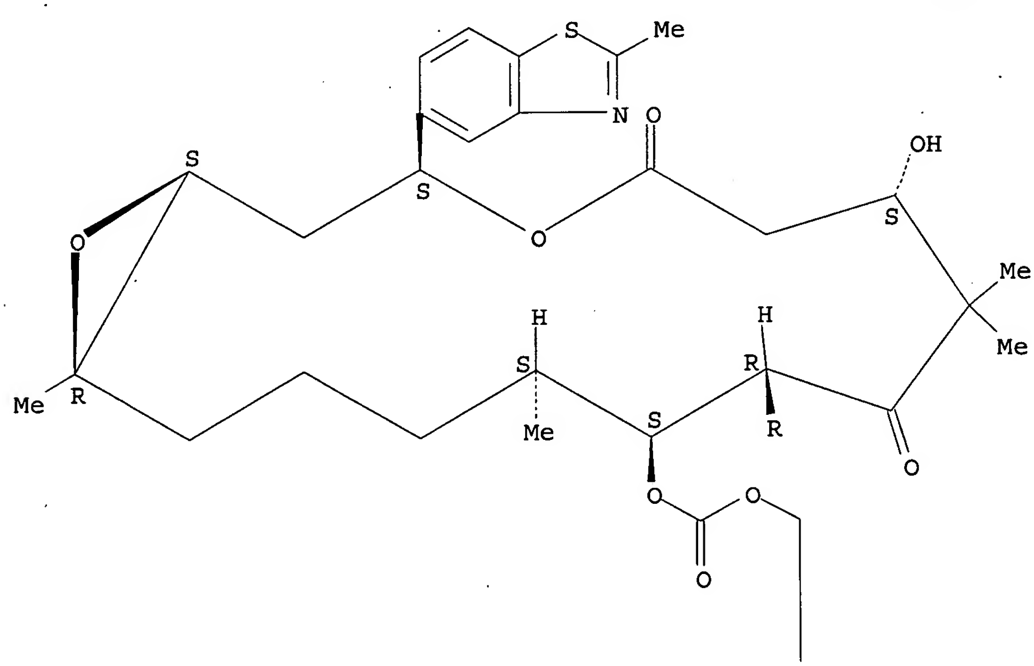
IT **658055-49-3DP**, sulfide conjugate with reduced AP39 antibody fragment
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new epothilone antibody peptide effector conjugates for pharmaceutical use in the treatment of proliferative or angiogenesis associated disease processes)

RN 658055-49-3 CAPLUS

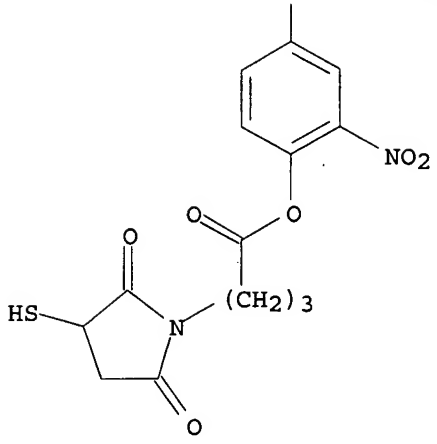
CN 1-Pyrrolidinebutanoic acid, 3-mercapto-2,5-dioxo-, 4-[[[[[(1S,3S,7S,10R,11S,12S,16R)-7-hydroxy-8,8,12,16-tetramethyl-3-(2-methyl-5-benzothiazolyl)-5,9-dioxo-10-(2-propenyl)-4,17-dioxabicyclo[14.1.0]heptadec-11-yl]oxy]carbonyl]oxy]methyl]-2-nitrophenyl ester (9CI) (CA INDEX NAME)

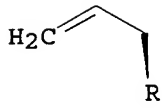
Absolute stereochemistry.

PAGE 1-A

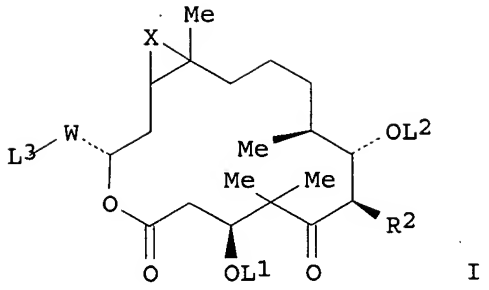


PAGE 2-A

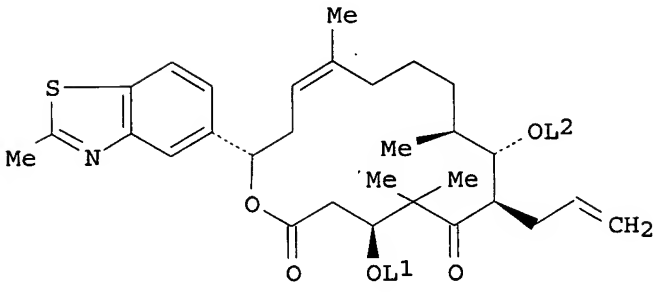




GI



I



II

AB Preparation of epothilone derivs., such as I (R2 = alkyl, alkenyl, alkynyl, aryl, etc.; L1, L2 = carboxyl, carbamoyl, carbonic linking group with a terminal group, such as maleimido, suitable for forming a sulfide link with a bio. mol.; L3 = heteroaryl, such as thiazol-4-yl; W = alkenylene

linking group; or L3W = heteroaryl, such as benzothiazol-5-yl; X = O, bond), as effectors linked with suitable biomols. as recognition units was described (no biol. testing data was presented). Production of the epothilone conjugates was carried out by the effectors being reacted with suitable linkers, and the compds. that were produced were conjugated to biomol. recognition units. These conjugates are claimed for use in the treatment of proliferative or angiogenesis-associated disease processes, such as tumors, inflammatory diseases, neurodegenerative diseases, such as multiple sclerosis and Alzheimer's disease, and rheumatoid arthritis. Thus, epothilone derivative II [L1 = 3-(2,5-dioxo-2,5-dihydropyrrol-1-yl)-1-Pr, L2 = H] was prepared via a carbamoylation of silylated epothilone I (L1 = H, L2 = SiMe2CMe3) with 3-(2,5-dioxo-2,5-dihydropyrrol-1-yl)-1-propylisocyanate and subsequent desilylation.

=>
Connection closed by remote host

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1201txs

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS	3	JUL 20	Powerful new interactive analysis and visualization software, STN AnaVist, now available
NEWS	4	AUG 11	Derwent World Patents Index(R) web-based training during August
NEWS	5	AUG 11	STN AnaVist workshops to be held in North America
NEWS	6	AUG 30	CA/CAplus -Increased access to 19th century research documents
NEWS	7	AUG 30	CASREACT - Enhanced with displayable reaction conditions
NEWS	8	SEP 09	ACD predicted properties enhanced in REGISTRY/ZREGISTRY

NEWS EXPRESS	JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 19:19:32 ON 21 SEP 2005

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:19:38 ON 21 SEP 2005
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STRUCTURE FILE UPDATES: 20 SEP 2005 HIGHEST RN 863546-28-5
DICTIONARY FILE UPDATES: 20 SEP 2005 HIGHEST RN 863546-28-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

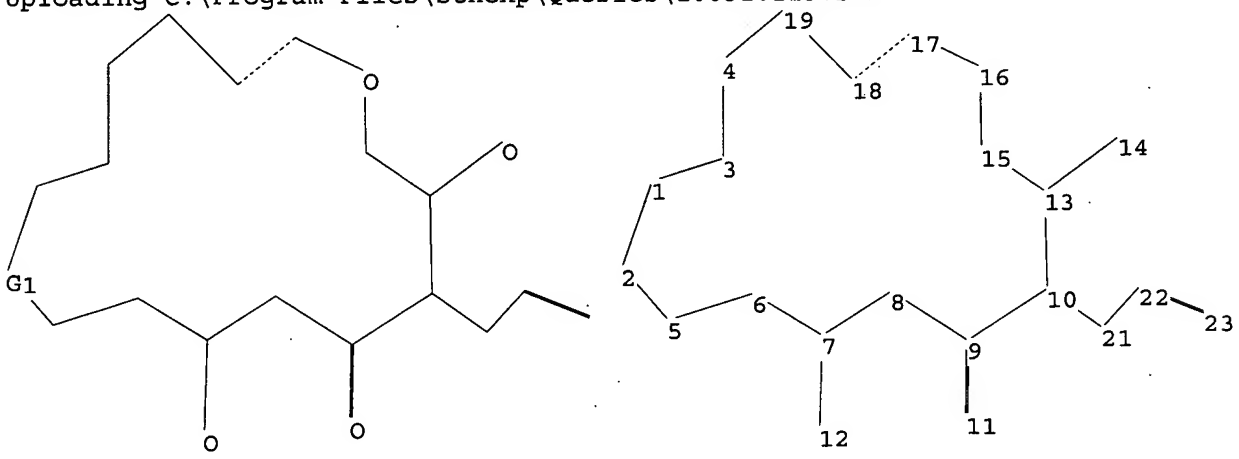
Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\106310113.str



chain nodes :
11 12 14 21 22 23
ring nodes :
1 2 3 4 5 6 7 8 9 10 13 15 16 17 18 19
chain bonds :
7-12 9-11 10-21 13-14 21-22 22-23
ring bonds :
1-2 1-3 2-5 3-4 4-19 5-6 6-7 7-8 8-9 9-10 10-13 13-15 15-16 16-17
17-18 18-19

exact/norm bonds :
1-2 1-3 2-5 3-4 4-19 5-6 6-7 7-8 7-12 8-9 9-10 9-11 10-13 10-21 13-14
13-15 15-16 16-17 17-18 18-19 21-22 22-23

G1:C,O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
21:CLASS 22:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 19:19:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1373 TO ITERATE

100.0% PROCESSED 1373 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 25238 TO 29682
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 ful
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FULL SCREEN SEARCH COMPLETED - 27838 TO ITERATE

100.0% PROCESSED 27838 ITERATIONS 56 ANSWERS
SEARCH TIME: 00.00.01

L3 56 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 19:20:14 ON 21 SEP 2005
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FILE COVERS 1907 - 21 Sep 2005 VOL 143 ISS 13
FILE LAST UPDATED: 20 Sep 2005 (20050920/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d l4 ibib hitstr abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:780372 CAPLUS
DOCUMENT NUMBER: 135:331295
TITLE: Preparation of oxa-epothilone derivatives for pharmaceutical use in the treatment of cancer
INVENTOR(S): Schwede, Wolfgang; Klar, Ulrich; Skuballa, Werner; Buchmann, Bernd; Hoffmann, Jens; Lichtner, Rosemarie
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 46 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 10020899	A1	20011025	DE 2000-10020899		20000420
WO 2001081341	A2	20011101	WO 2001-EP4551		20010419
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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PRIORITY APPLN. INFO.:			DE 2000-10020899	A	20000420
			WO 2001-EP4551	W	20010419

OTHER SOURCE(S): MARPAT 135:331295
IT **369639-83-8P 369639-89-4P 369639-96-3P**
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369640-84-6P 369640-90-4P 369640-97-1P
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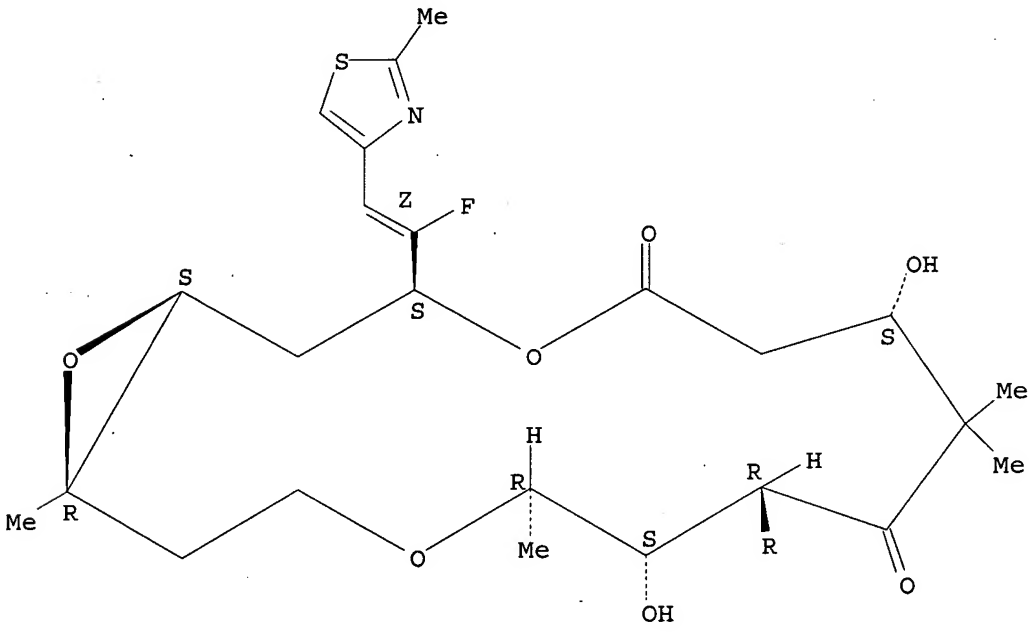
369642-59-1P 369642-63-7P 369642-82-0P
369642-86-4P 369642-90-0P 369642-94-4P
369643-19-6P 369643-20-9P 369643-69-6P
369643-70-9P 369643-94-7P 369643-95-8P
369644-51-9P 369644-52-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of oxa-epothilone derivs. for pharmaceutical use in the treatment of cancer)

RN 369639-83-8 CAPLUS

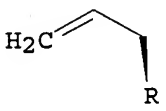
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 3-[(1Z)-1-fluoro-2-(2-methyl-4-thiazolyl)ethenyl]-7,11-dihydroxy-8,8,12,16-tetramethyl-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 2-A

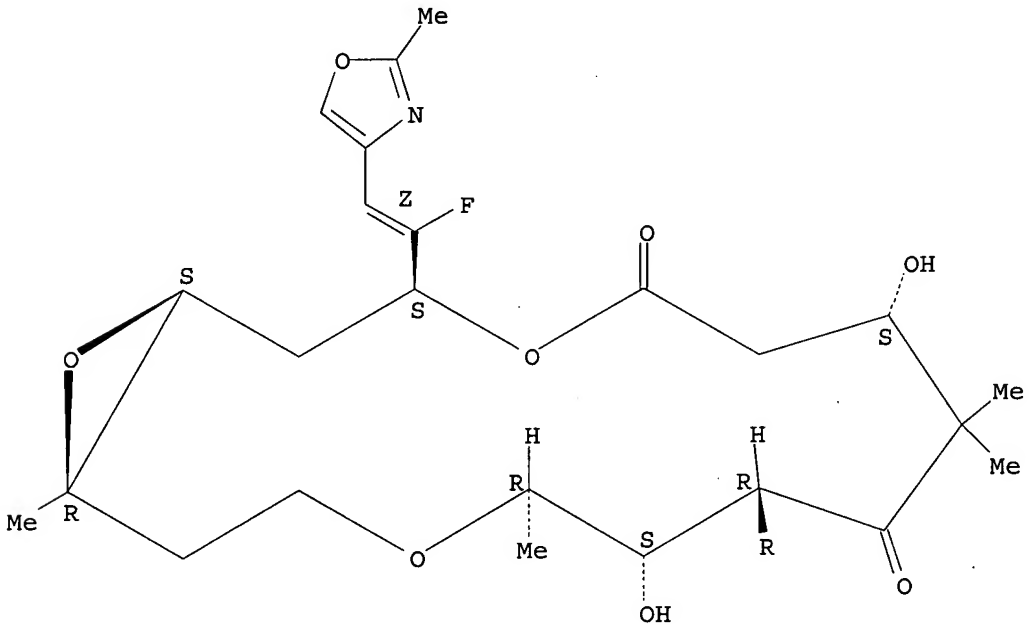


RN 369639-89-4 CAPLUS

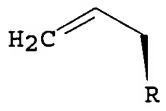
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 3-[(1Z)-1-fluoro-2-(2-methyl-4-oxazolyl)ethenyl]-7,11-dihydroxy-8,8,12,16-tetramethyl-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



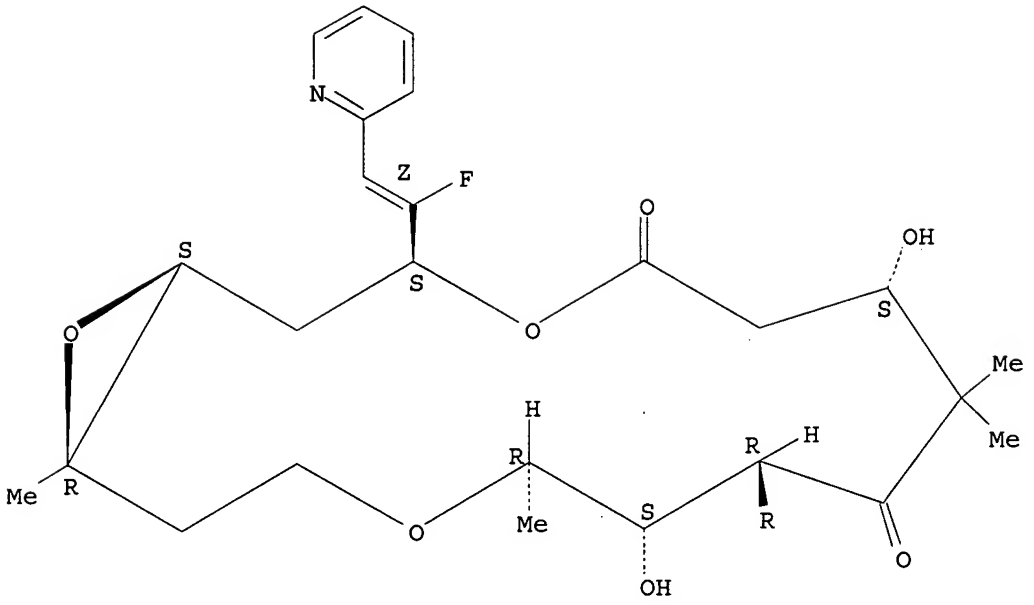
PAGE 2-A



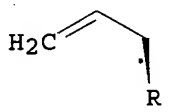
RN 369639-96-3 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 3-[(1Z)-1-fluoro-2-(2-pyridinyl)ethenyl]-7,11-dihydroxy-8,8,12,16-tetramethyl-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



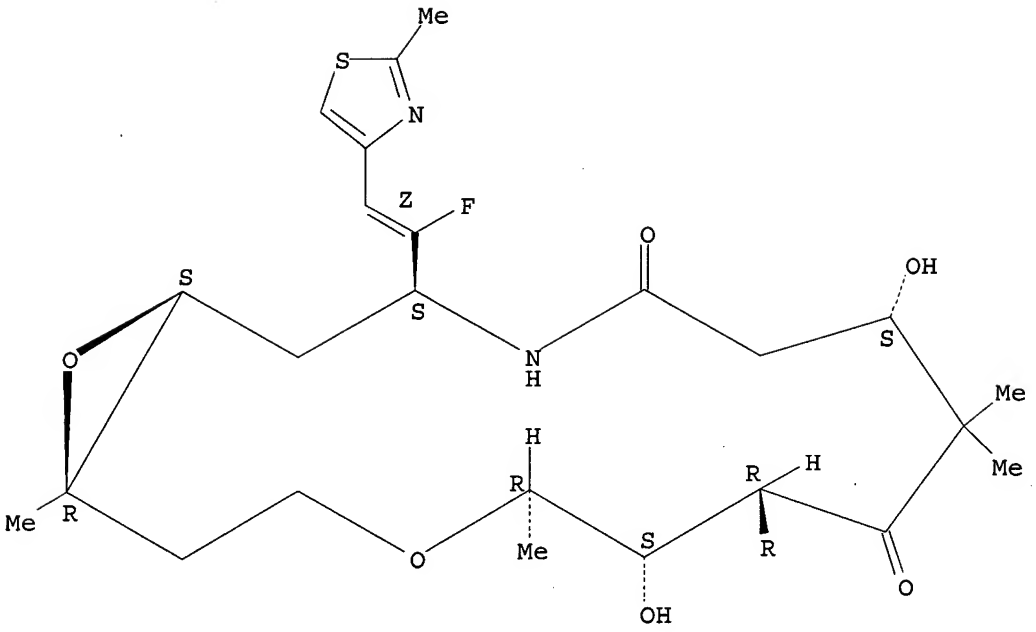
PAGE 2-A



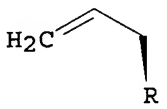
RN 369640-03-9 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 14-[(1Z)-1-fluoro-2-(2-methyl-4-thiazolyl)ethenyl]-6,10-dihydroxy-1,5,9,9-tetramethyl-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



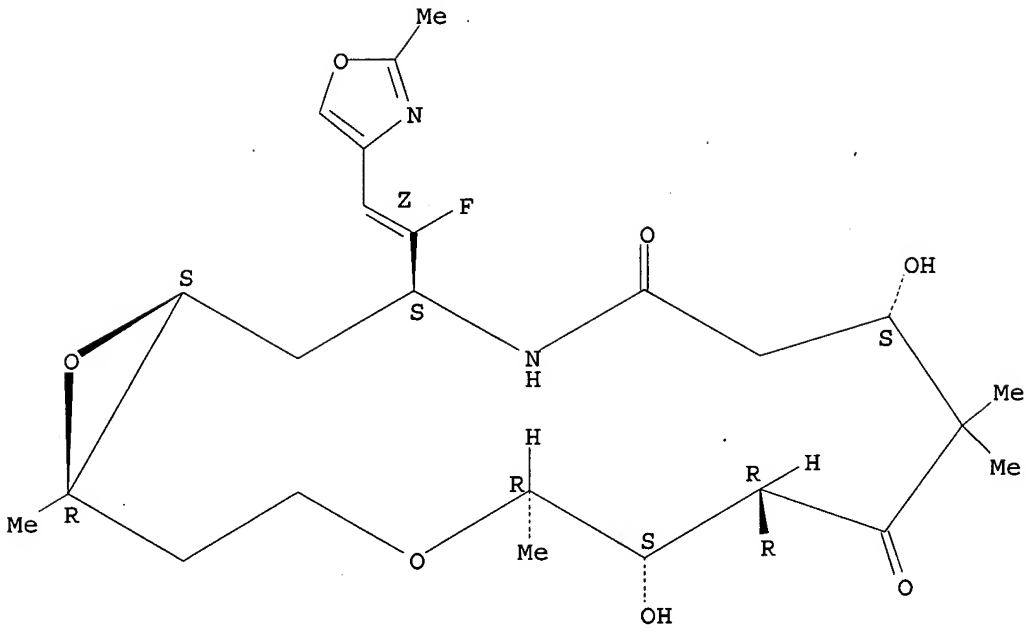
PAGE 2-A



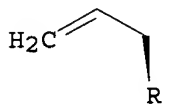
RN 369640-10-8 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 14-[(1Z)-1-fluoro-2-(2-methyl-4-oxazolyl)ethenyl]-6,10-dihydroxy-1,5,9,9-tetramethyl-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



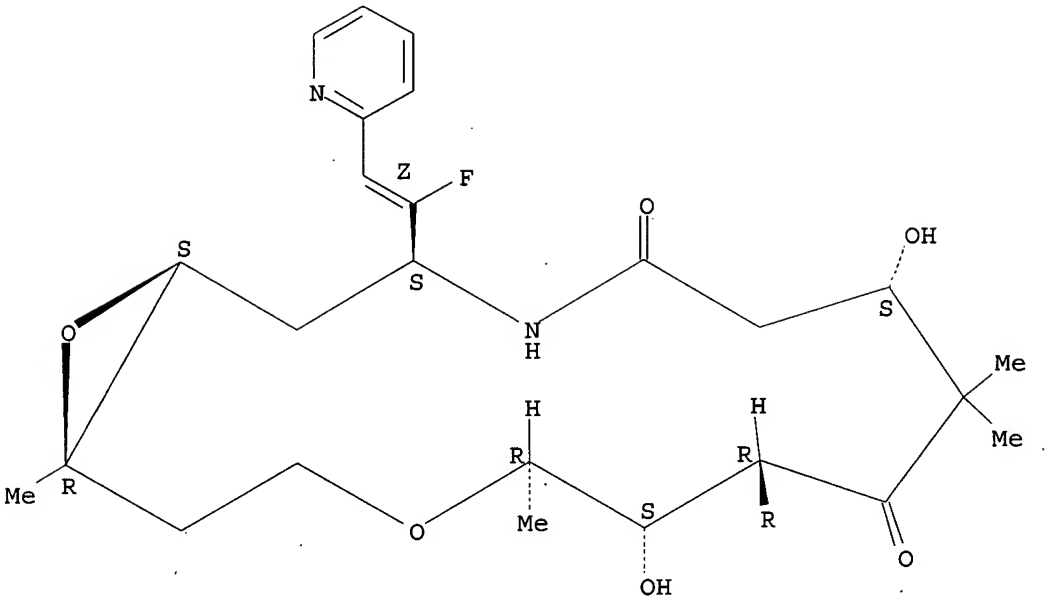
PAGE 2-A



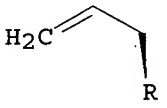
RN 369640-20-0 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 14-[(1Z)-1-fluoro-2-(2-pyridinyl)ethenyl]-6,10-dihydroxy-1,5,9,9-tetramethyl-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



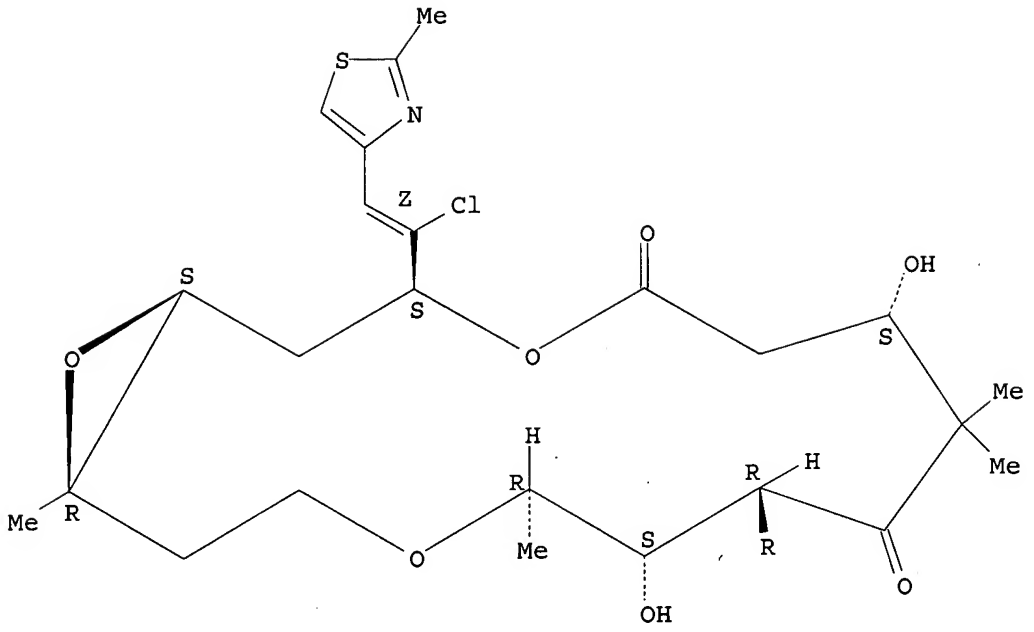
PAGE 2-A



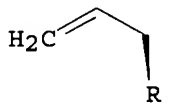
RN 369640-32-4 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 3-[(1Z)-1-chloro-2-(2-methyl-4-thiazolyl)ethenyl]-7,11-dihydroxy-8,8,12,16-tetramethyl-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



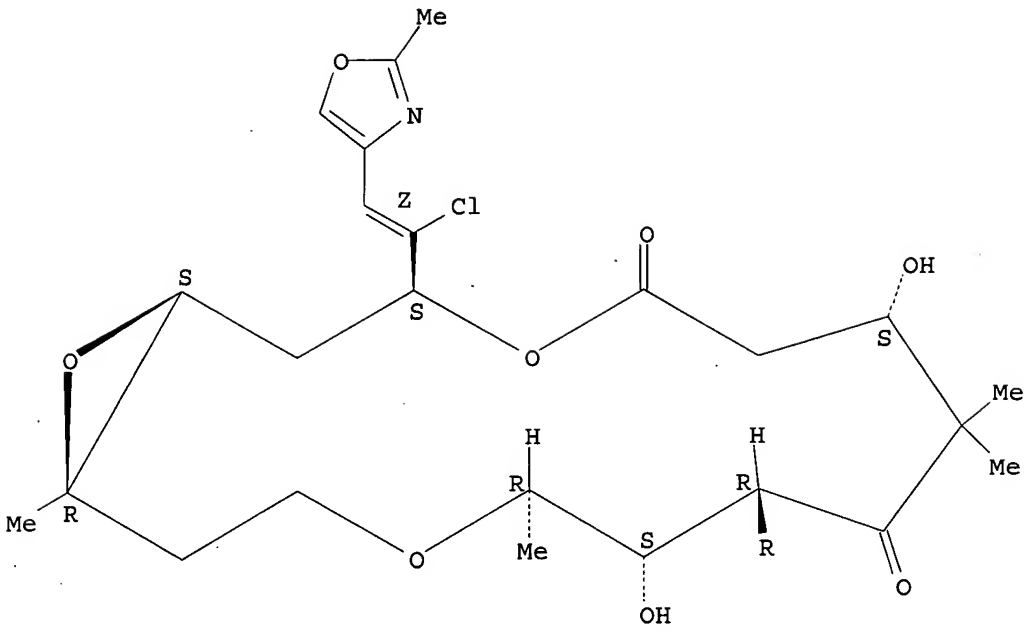
PAGE 2-A



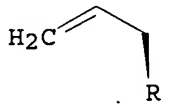
RN 369640-43-7 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 3-[(1Z)-1-chloro-2-(2-methyl-4-oxazolyl)ethenyl]-7,11-dihydroxy-8,8,12,16-tetramethyl-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



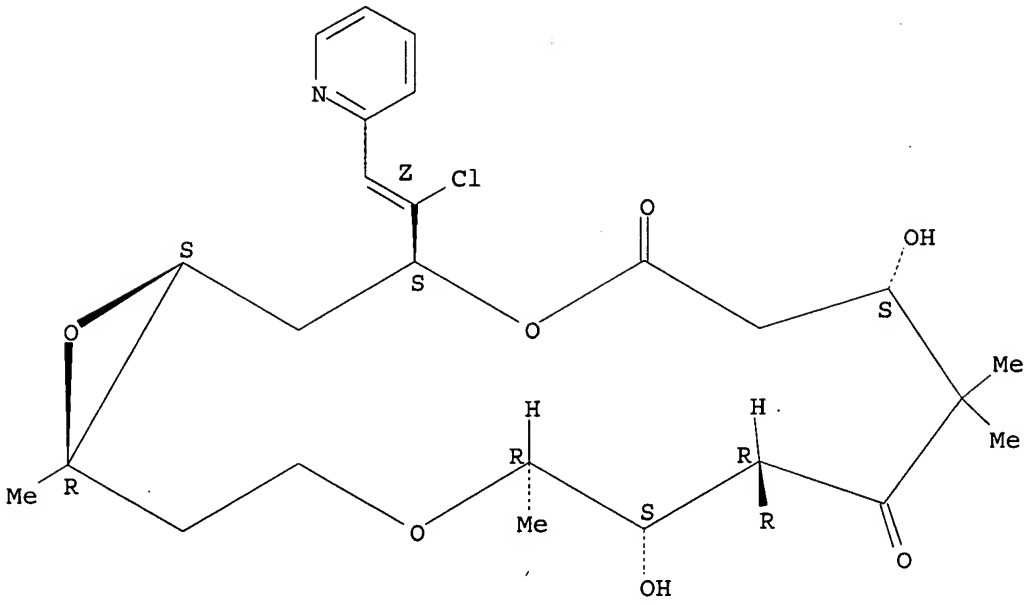
PAGE 2-A



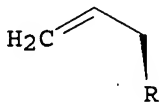
RN 369640-56-2 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 3-[(1Z)-1-chloro-2-(2-pyridinyl)ethenyl]-7,11-dihydroxy-8,8,12,16-tetramethyl-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



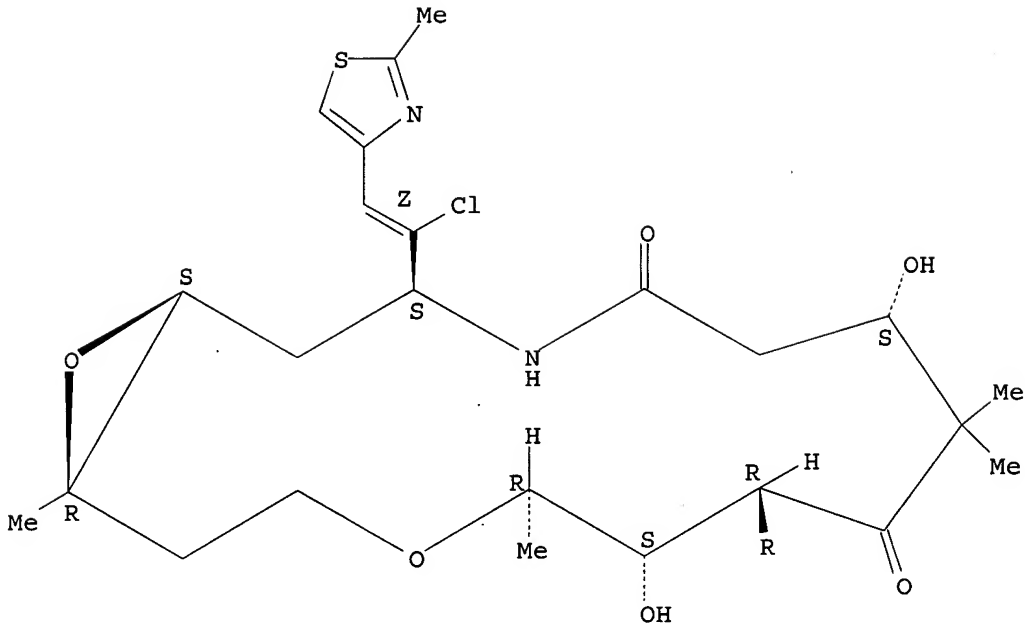
PAGE 2-A



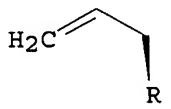
RN 369640-65-3 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 14-[(1Z)-1-chloro-2-(2-methyl-4-thiazolyl)ethenyl]-6,10-dihydroxy-1,5,9,9-tetramethyl-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



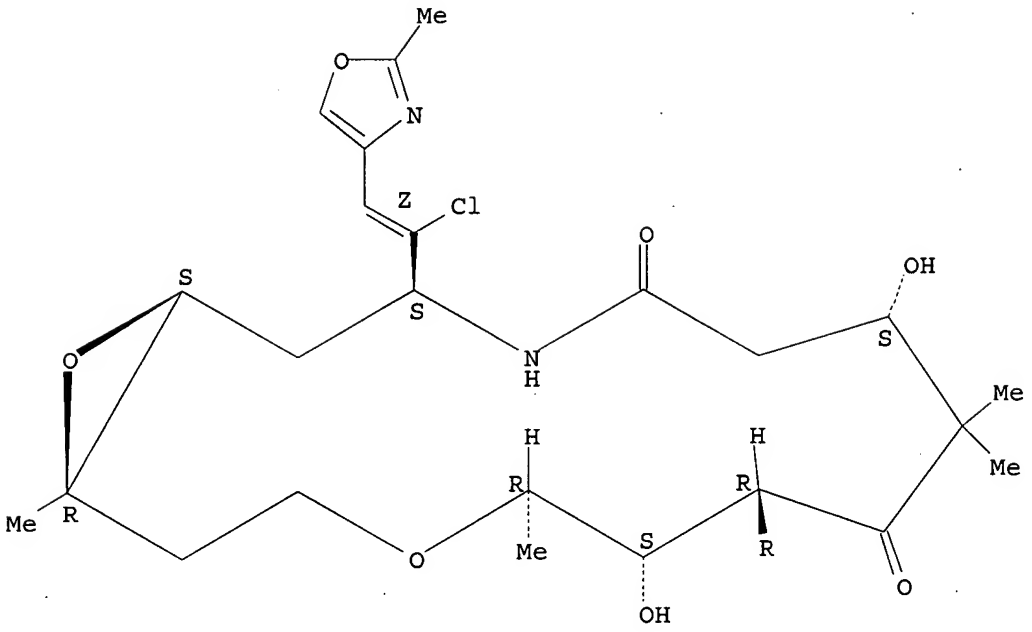
PAGE 2-A



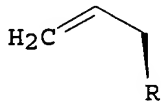
RN 369640-72-2 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 14-[(1Z)-1-chloro-2-(2-methyl-4-oxazolyl)ethenyl]-6,10-dihydroxy-1,5,9,9-tetramethyl-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



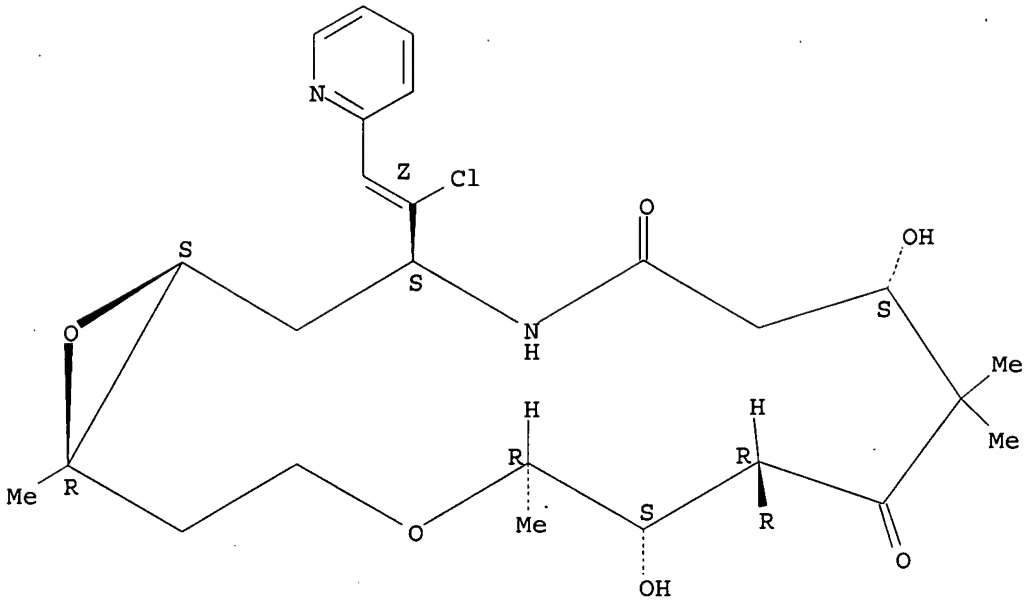
PAGE 2-A



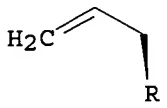
RN 369640-78-8 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 14-[(1Z)-1-chloro-2-(2-pyridinyl)ethenyl]-6,10-dihydroxy-1,5,9,9-tetramethyl-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



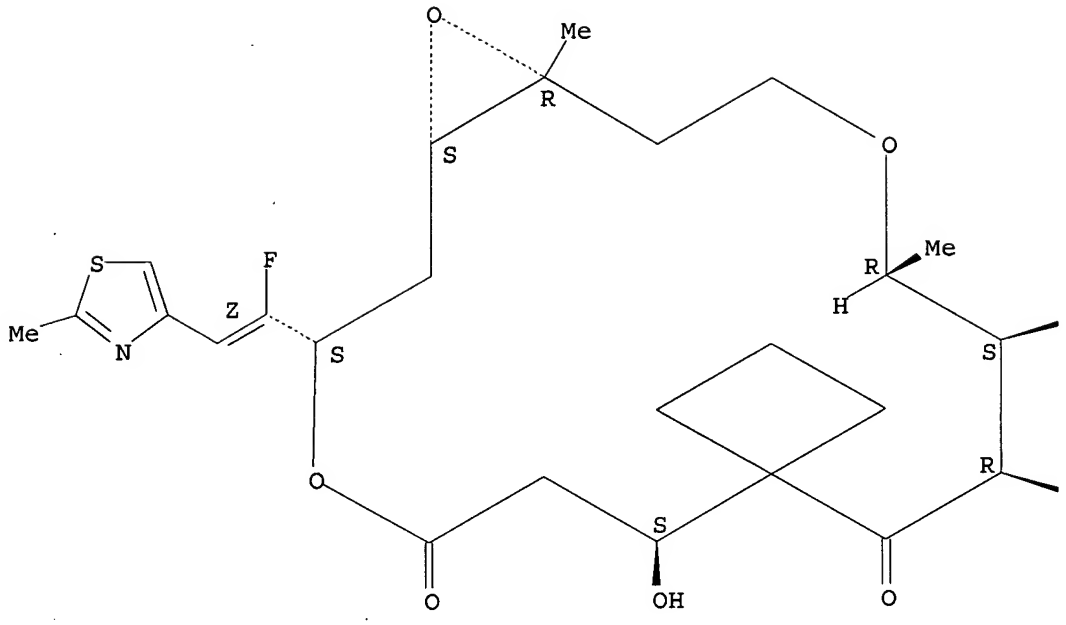
PAGE 2-A



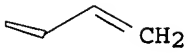
RN 369640-84-6 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 3'-[(1Z)-1-fluoro-2-(2-methyl-4-thiazolyl)ethenyl]-7',11'-dihydroxy-12',16'-dimethyl-10'-(2-propenyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



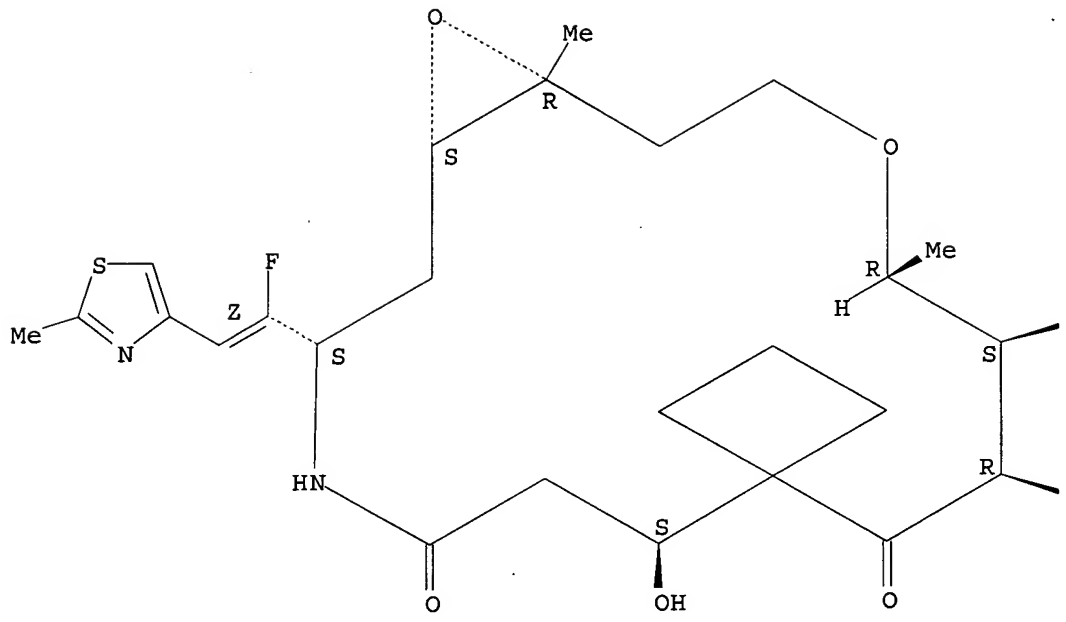
PAGE 1-B



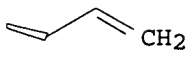
RN 369640-90-4 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 14'-[(1Z)-1-fluoro-2-(2-methyl-4-thiazolyl)ethenyl]-6',10'-dihydroxy-1',5'-dimethyl-7'-(2-propenyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



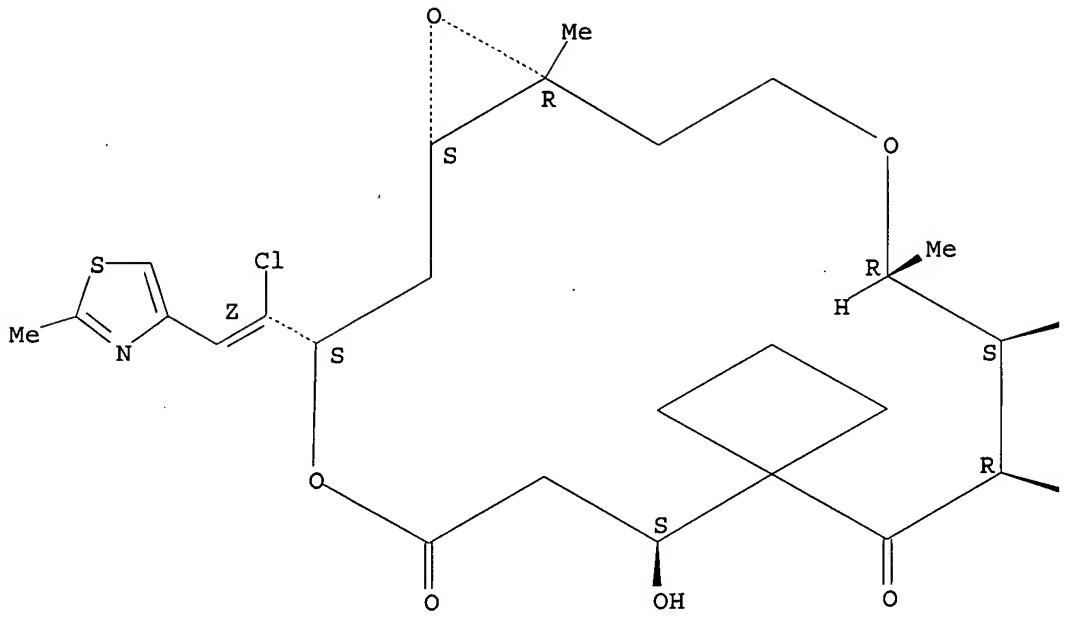
PAGE 1-B



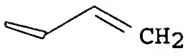
RN 369640-97-1 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 3'-[(1Z)-1-chloro-2-(2-methyl-4-thiazolyl)ethenyl]-7',11'-dihydroxy-12',16'-dimethyl-10'-(2-propenyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



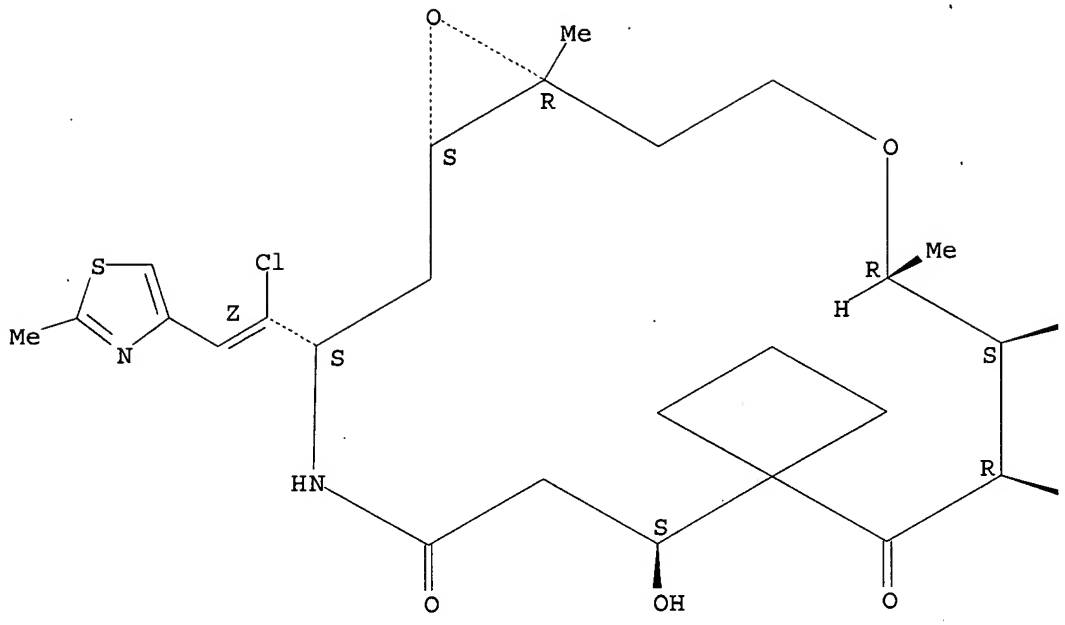
PAGE 1-B



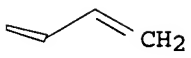
RN 369641-03-2 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 14'-[(1Z)-1-chloro-2-(2-methyl-4-thiazolyl)ethenyl]-6',10'-dihydroxy-1',5'-dimethyl-7'-(2-propenyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

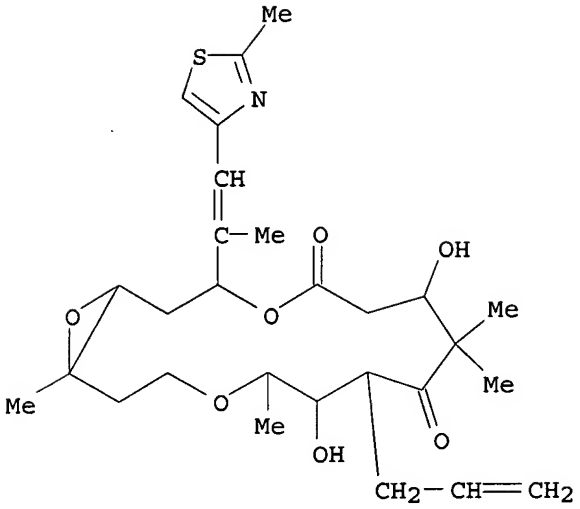
PAGE 1-A



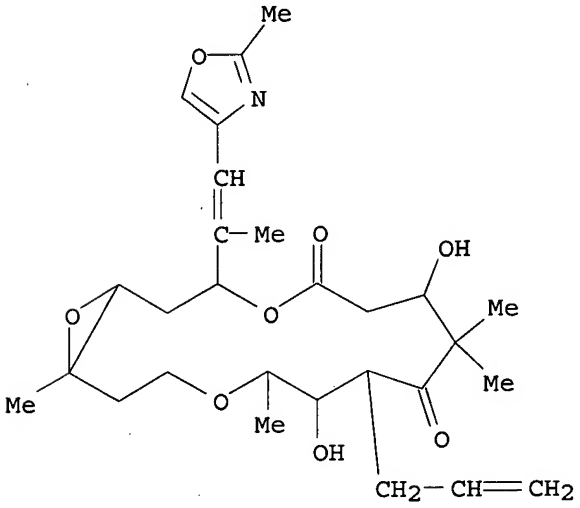
PAGE 1-B



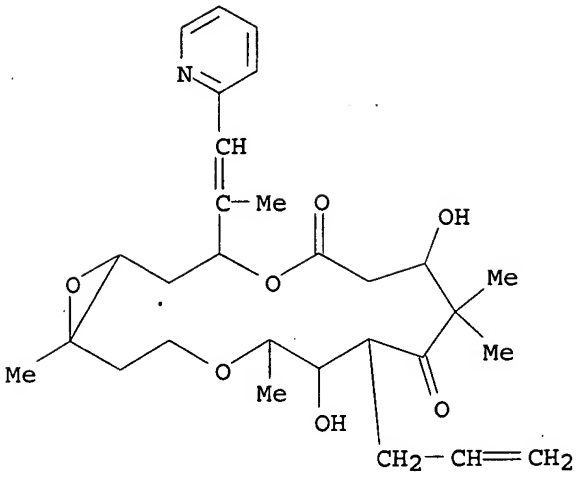
RN 369641-05-4 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 7,11-dihydroxy-8,8,12,16-tetramethyl-3-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)



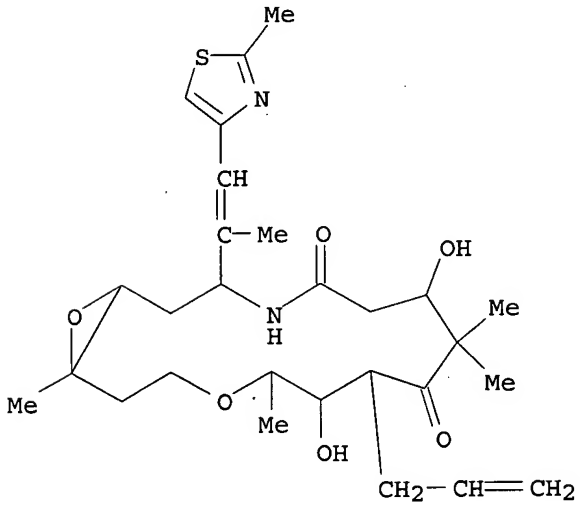
RN 369641-07-6 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 7,11-dihydroxy-8,8,12,16-tetramethyl-3-[(1Z)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl]-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)



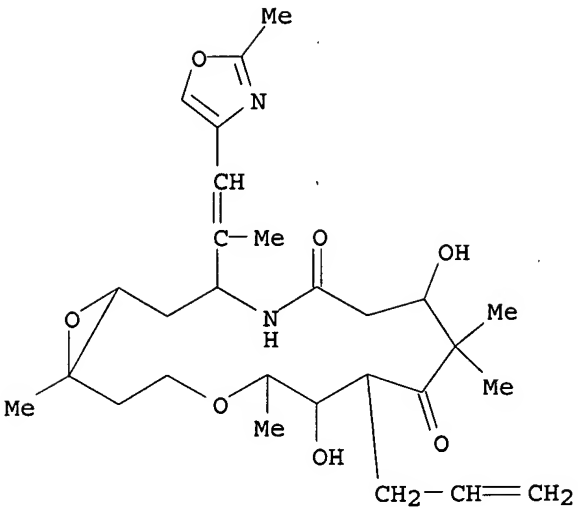
RN 369641-09-8 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 7,11-dihydroxy-8,8,12,16-tetramethyl-3-[(1Z)-1-methyl-2-(2-pyridinyl)ethenyl]-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)



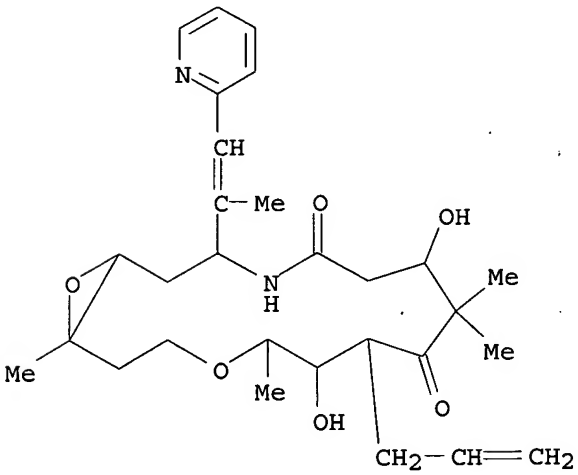
RN 369641-11-2 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 6,10-dihydroxy-1,5,9,9-tetramethyl-14-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)



RN 369641-13-4 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 6,10-dihydroxy-1,5,9,9-tetramethyl-14-[(1Z)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl]-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)



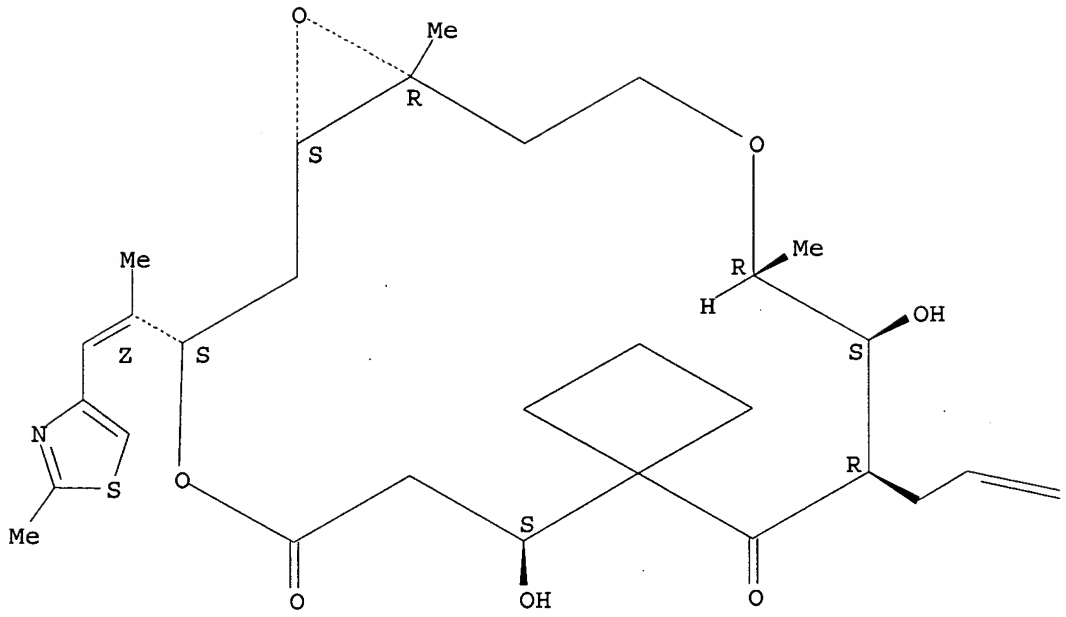
RN 369641-15-6 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 6,10-dihydroxy-1,5,9,9-tetramethyl-14-[(1Z)-1-methyl-2-(2-pyridinyl)ethenyl]-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)



RN 369641-17-8 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 7',11'-dihydroxy-12',16'-dimethyl-3'-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-10'-(2-propenyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



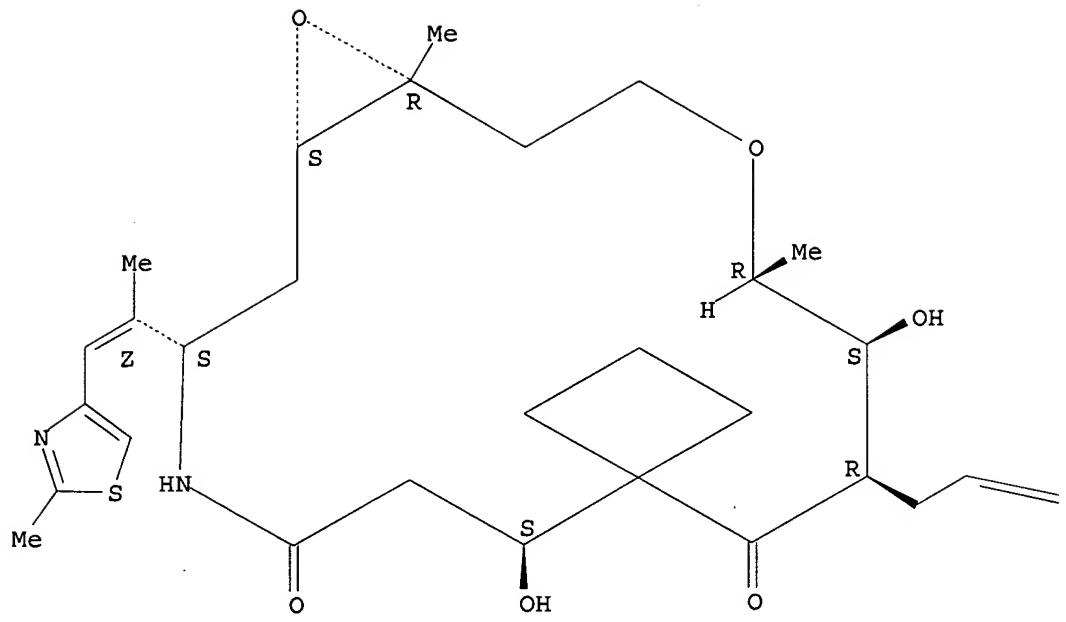
PAGE 1-B

$=CH_2$

RN 369641-19-0 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 6',10'-dihydroxy-1',5'-dimethyl-14'-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-7'-(2-propenyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

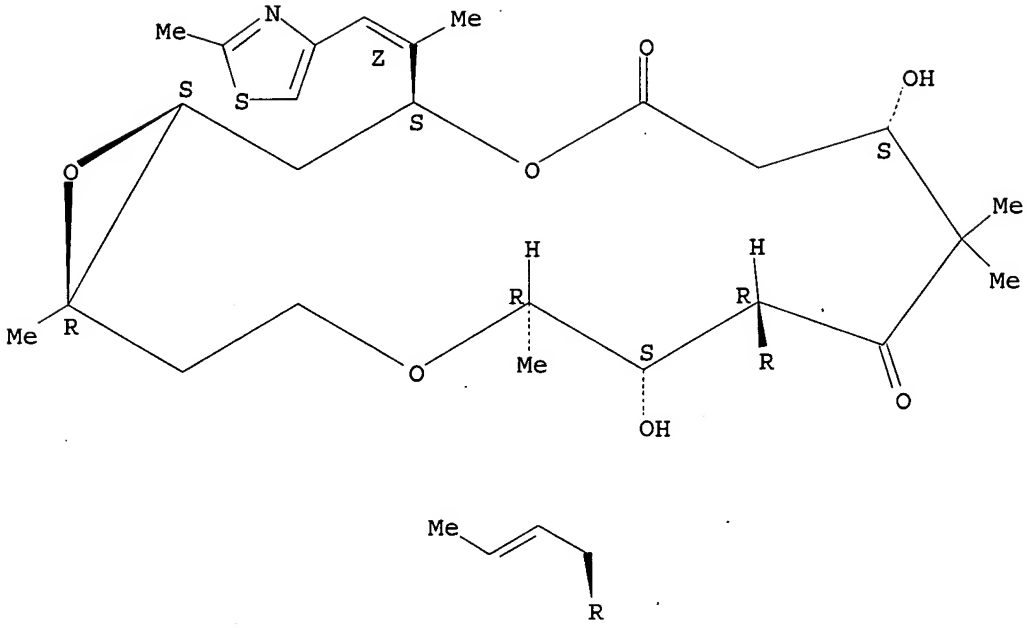


PAGE 1-B

$=CH_2$

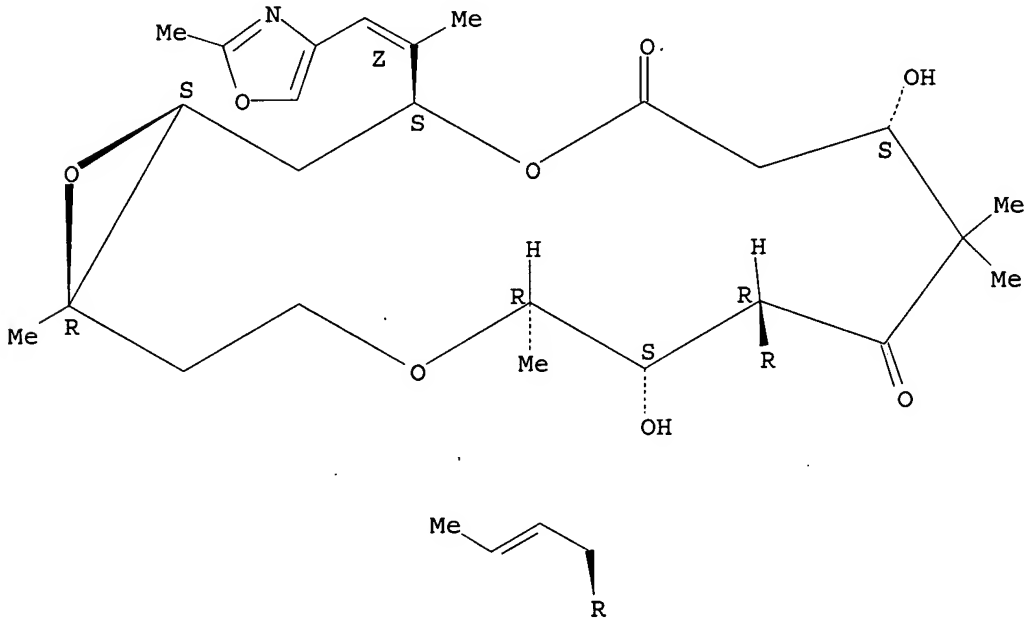
RN 369641-38-3 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 10-(2-butenyl)-7,11-dihydroxy-8,8,12,16-tetramethyl-3-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



RN 369641-42-9 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 10-(2-butenyl)-7,11-dihydroxy-8,8,12,16-tetramethyl-3-[(1Z)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl]-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

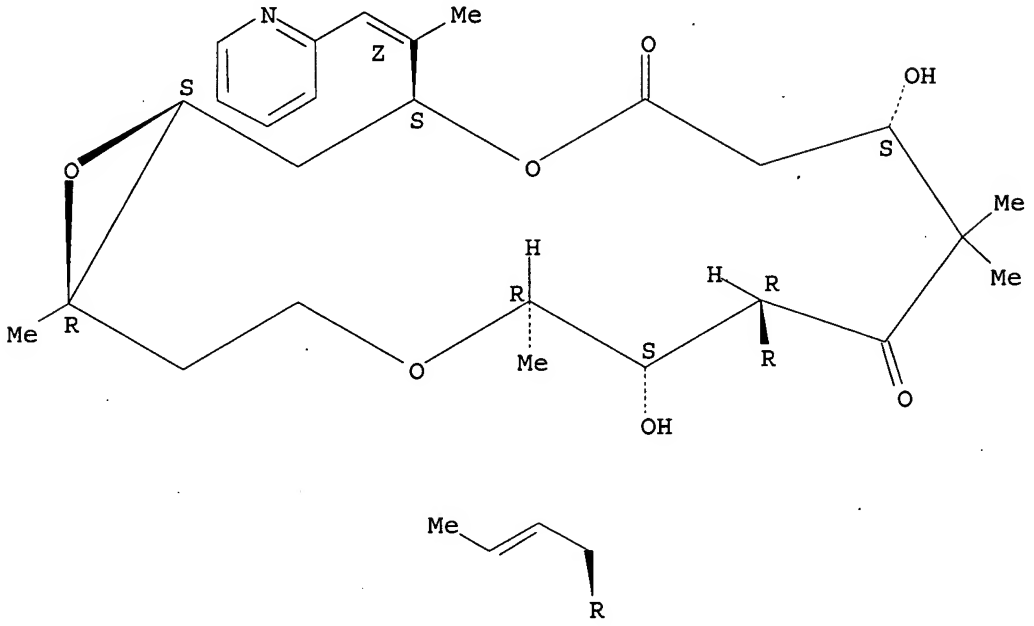
Absolute stereochemistry.
Double bond geometry as described by E or Z.



RN 369641-45-2 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 10-(2-butenyl)-7,11-dihydroxy-8,8,12,16-tetramethyl-3-[(1Z)-1-methyl-2-(2-pyridinyl)ethenyl]-,

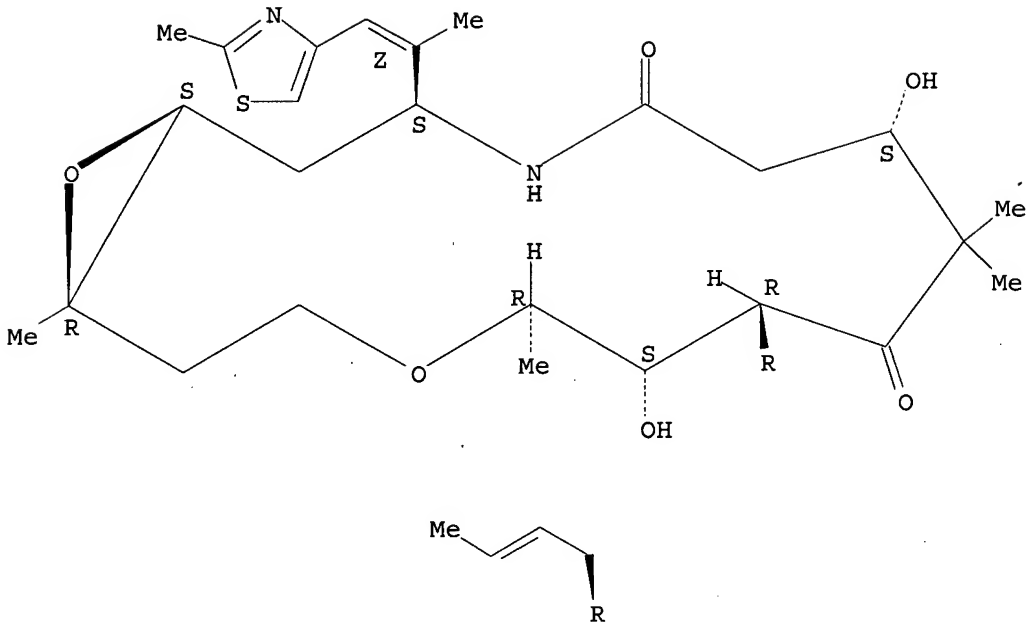
(1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



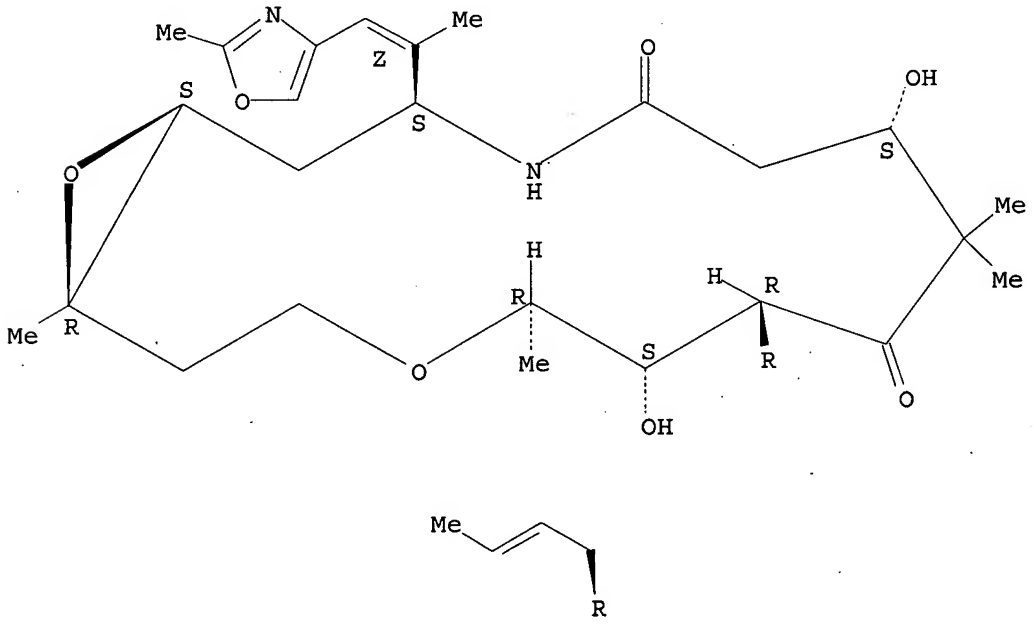
RN 369641-49-6 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 7-(2-butenyl)-6,10-dihydroxy-1,5,9,9-tetramethyl-14-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



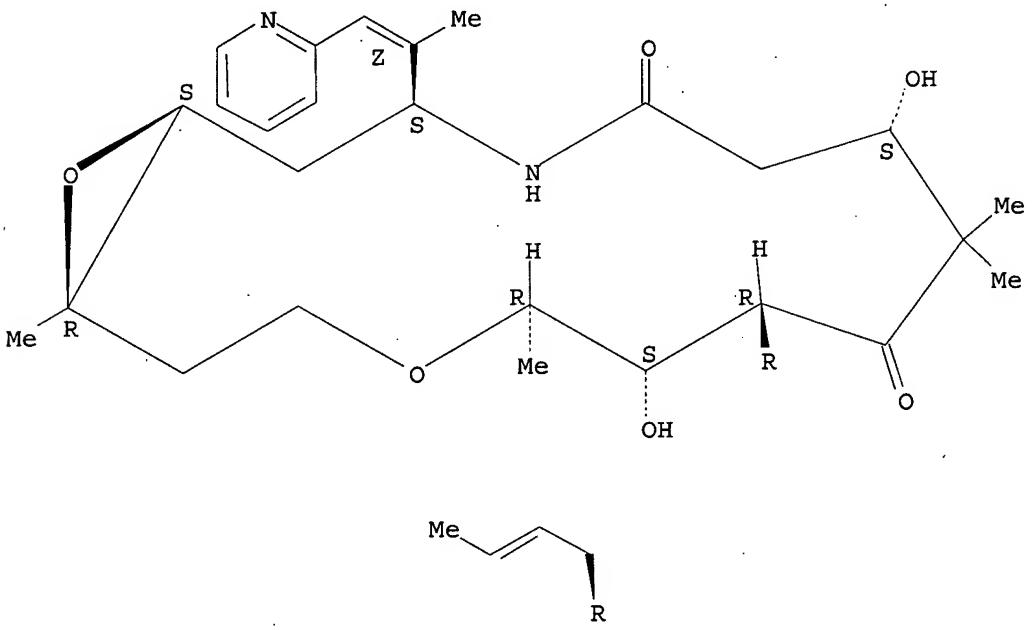
RN 369641-52-1 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 7-(2-butenyl)-6,10-dihydroxy-1,5,9,9-tetramethyl-14-[(1Z)-1-methyl-2-(2-methyl-4-oxazolyl)ethenyl]-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



RN 369641-56-5 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 7-(2-butenyl)-6,10-dihydroxy-1,5,9,9-tetramethyl-14-[(1Z)-1-methyl-2-(2-pyridinyl)ethenyl]-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

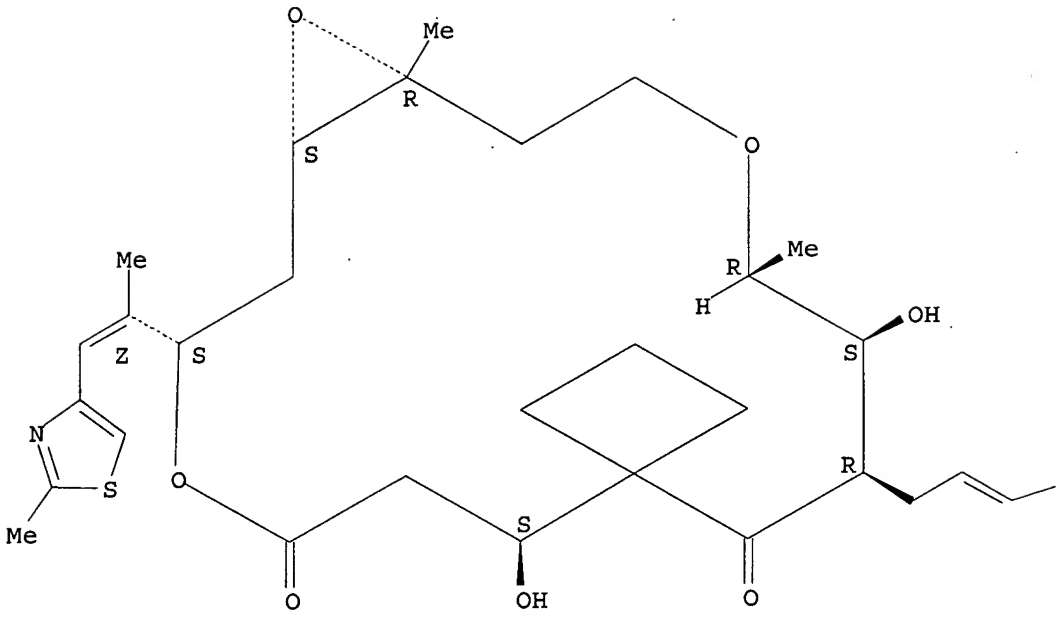
Absolute stereochemistry.
Double bond geometry as described by E or Z.



RN 369641-60-1 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 10'-(2-butenyl)-7',11'-dihydroxy-12',16'-dimethyl-3'-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A

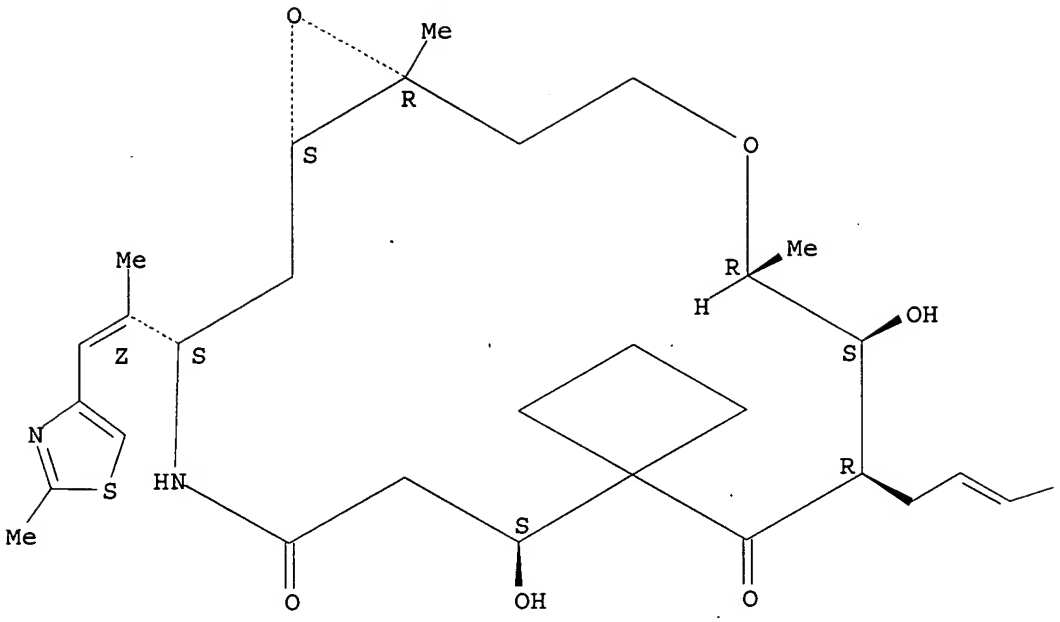


PAGE 1-B

RN 369641-63-4 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 7'-(2-butenyl)-6',10'-dihydroxy-1',5'-dimethyl-14'-[(1Z)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A



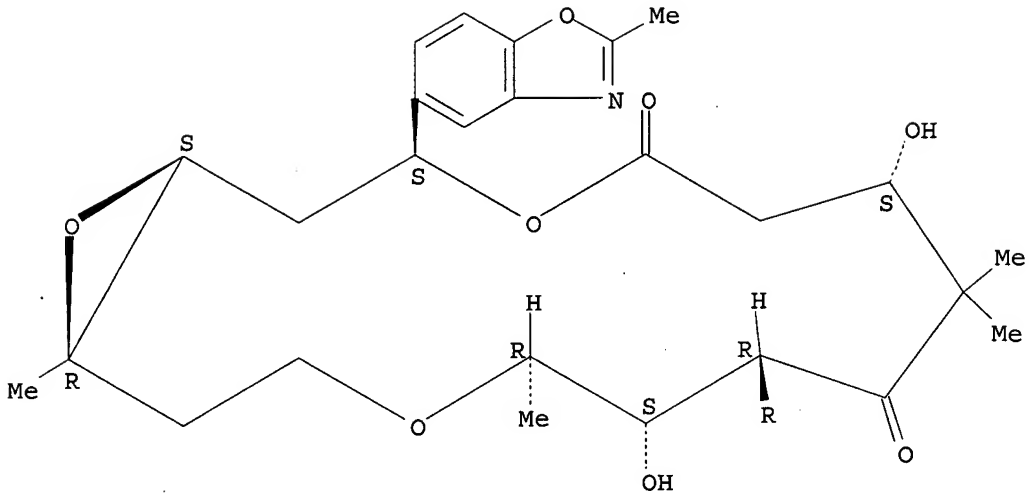
PAGE 1-B

Me

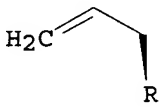
RN 369641-81-6 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 7,11-dihydroxy-8,8,12,16-tetramethyl-3-(2-methyl-5-benzoxazolyl)-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



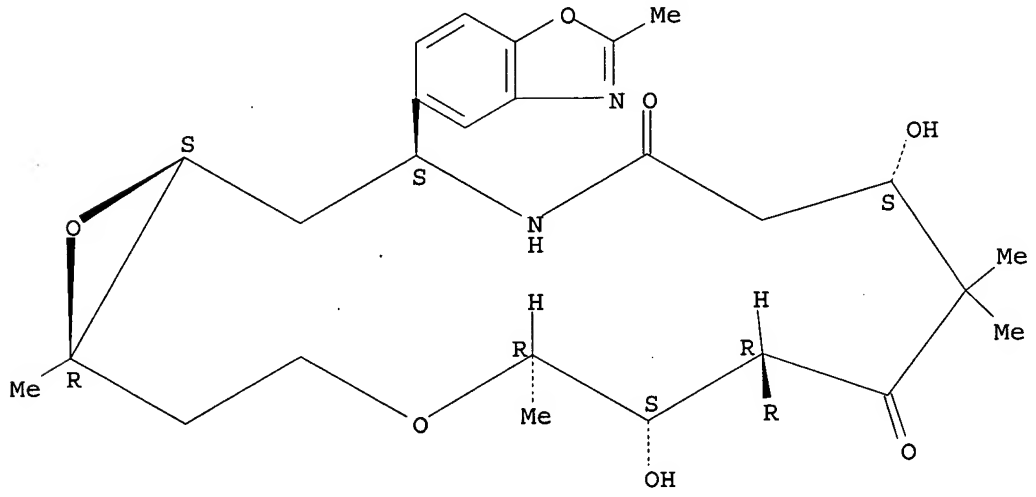
PAGE 2-A



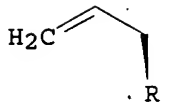
RN 369641-87-2 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 6,10-dihydroxy-1,5,9,9-tetramethyl-14-(2-methyl-5-benzoxazolyl)-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



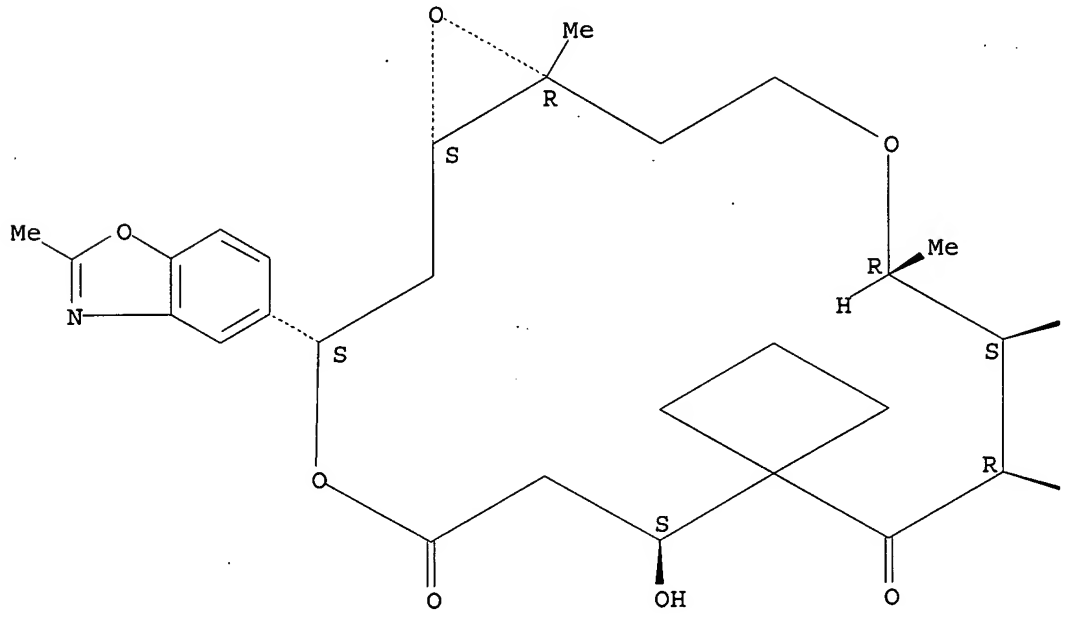
PAGE 2-A



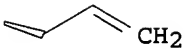
RN 369641-92-9 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 7',11'-dihydroxy-12',16'-dimethyl-3'-(2-methyl-5-benzoxazolyl)-10'-(2-propenyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



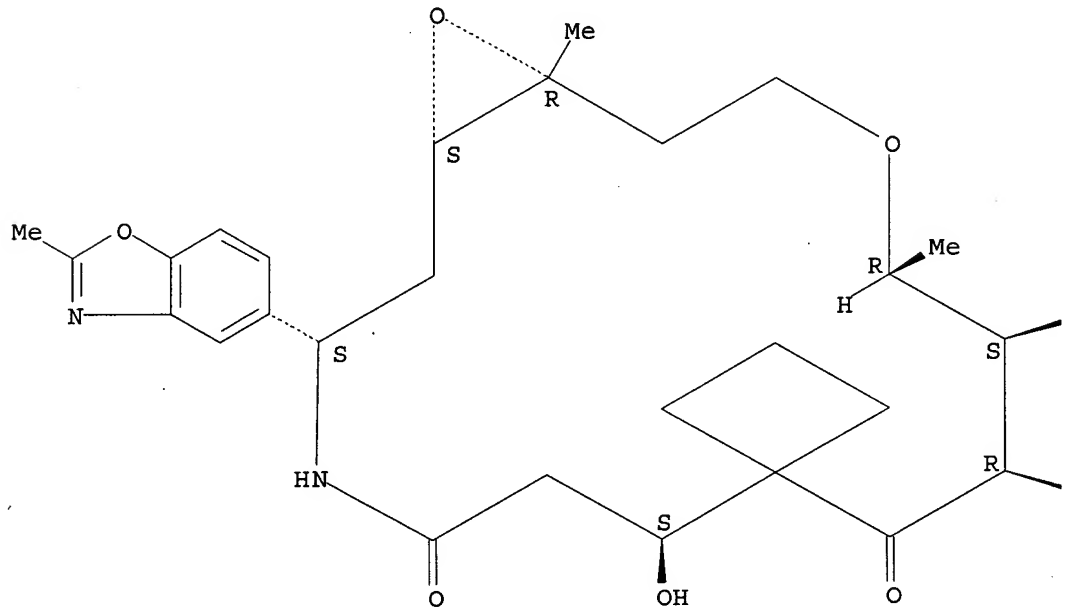
PAGE 1-B

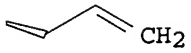


RN 369641-96-3 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 6',10'-dihydroxy-1',5'-dimethyl-14'-(2-methyl-5-benzoxazolyl)-7'-(2-propenyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

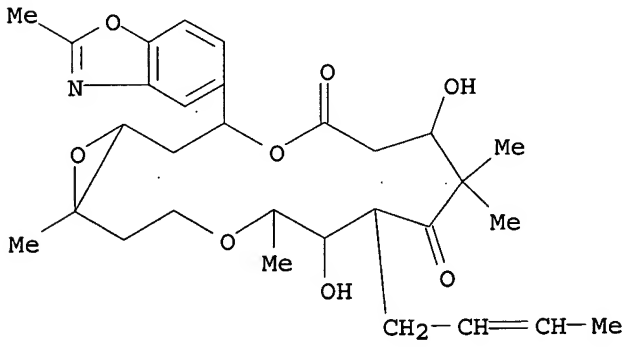
Absolute stereochemistry.

PAGE 1-A

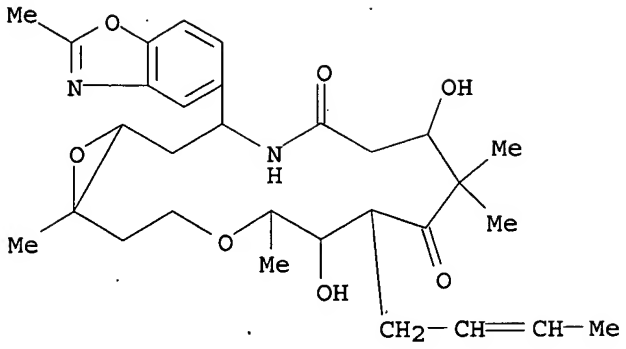




RN 369642-18-2 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 10-(2-butenyl)-7,11-dihydroxy-8,8,12,16-tetramethyl-3-(2-methyl-5-benzoxazolyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)



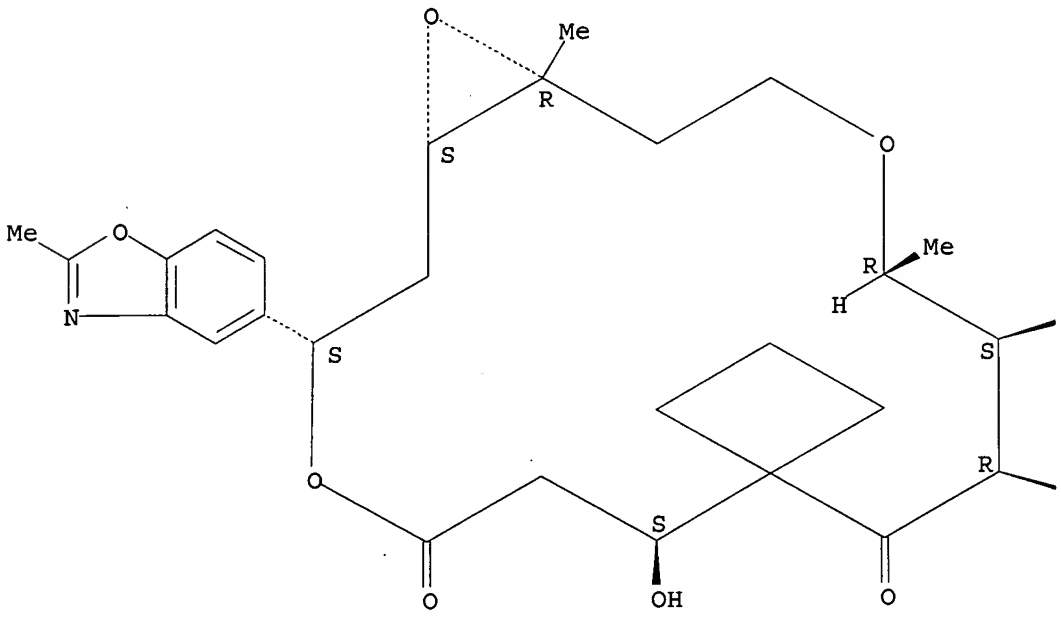
RN 369642-22-8 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 7-(2-butenyl)-6,10-dihydroxy-1,5,9,9-tetramethyl-14-(2-methyl-5-benzoxazolyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)



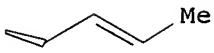
RN 369642-26-2 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 10'-(2-butenyl)-7',11'-dihydroxy-12',16'-dimethyl-3'-(2-methyl-5-benzoxazolyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



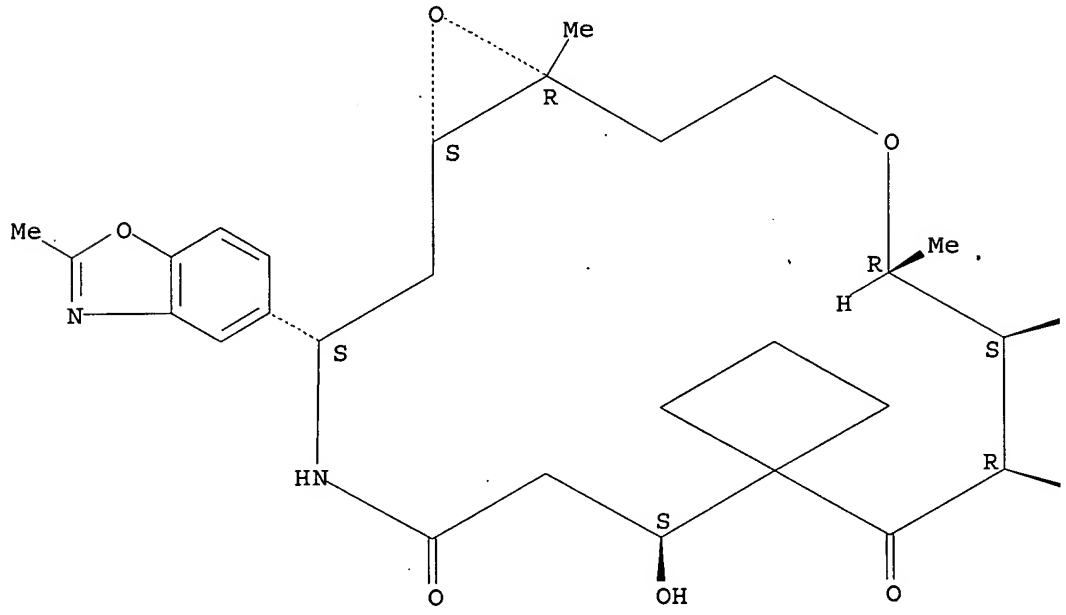
PAGE 1-B



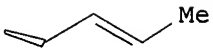
RN 369642-31-9 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 7'-(2-butenyl)-6',10'-dihydroxy-1',5'-dimethyl-14'-(2-methyl-5-benzoxazolyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



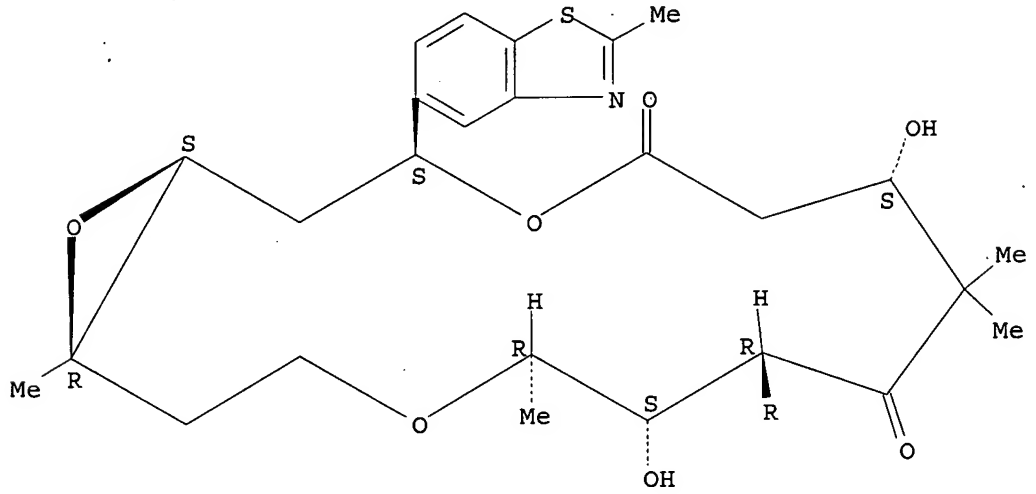
PAGE 1-B



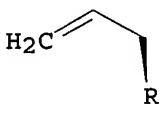
RN 369642-51-3 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 7,11-dihydroxy-8,8,12,16-tetramethyl-3-(2-methyl-5-benzothiazolyl)-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

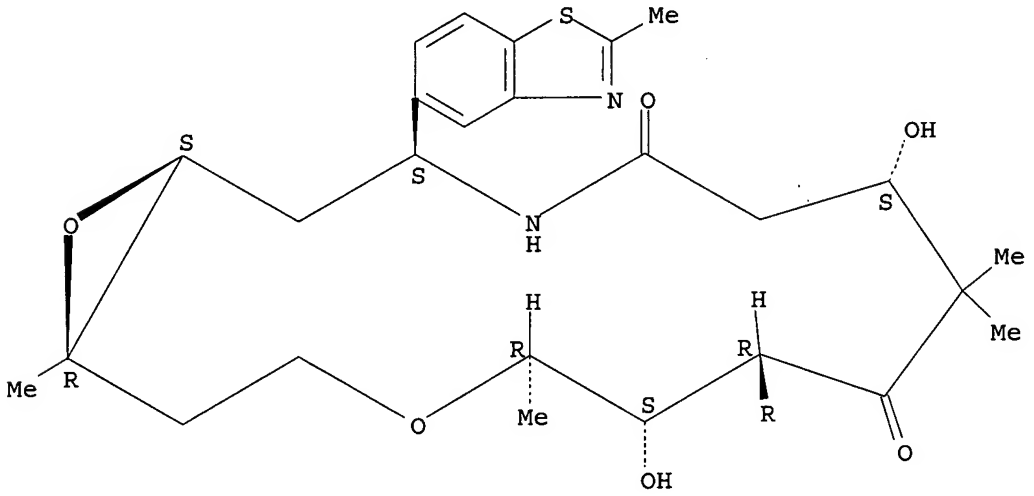


RN 369642-55-7 CAPLUS

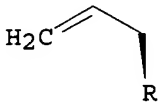
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 6,10-dihydroxy-1,5,9,9-tetramethyl-14-(2-methyl-5-benzothiazolyl)-7-(2-propenyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

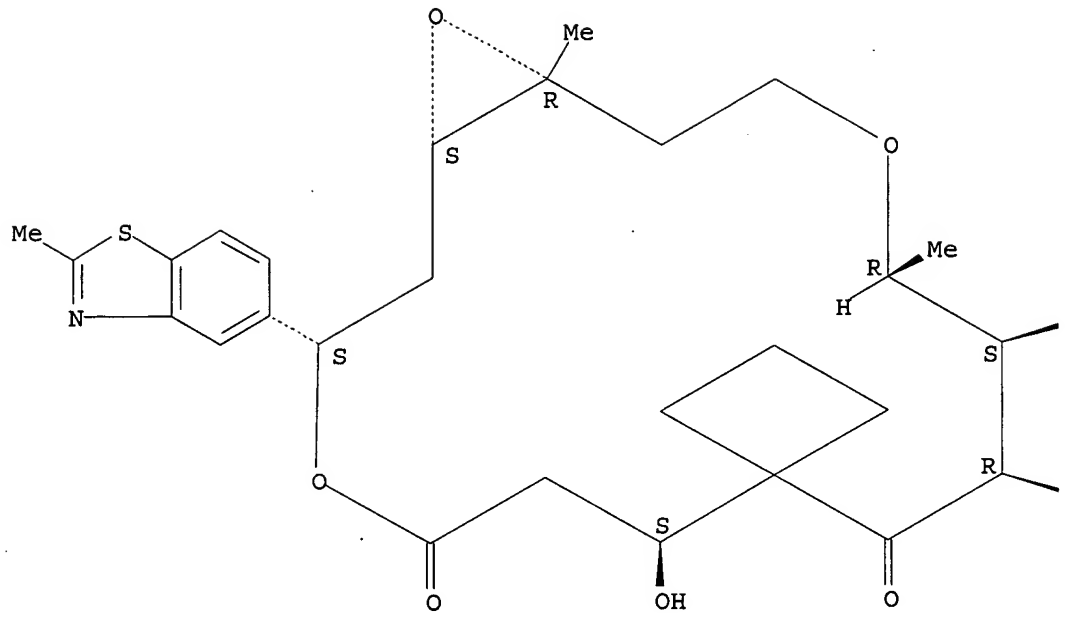


RN 369642-59-1 CAPLUS

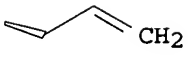
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 7',11'-dihydroxy-12',16'-dimethyl-3'-(2-methyl-5-benzothiazolyl)-10'-(2-propenyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



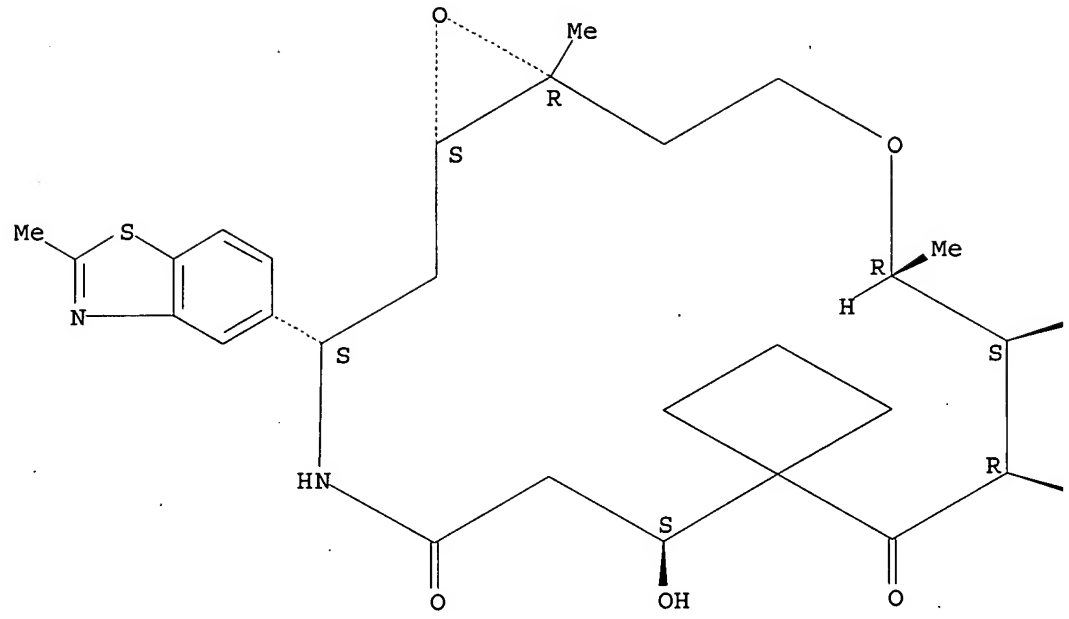
PAGE 1-B



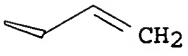
RN 369642-63-7 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 6',10'-dihydroxy-1',5'-dimethyl-14'-(2-methyl-5-benzothiazolyl)-7'-(2-propenyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



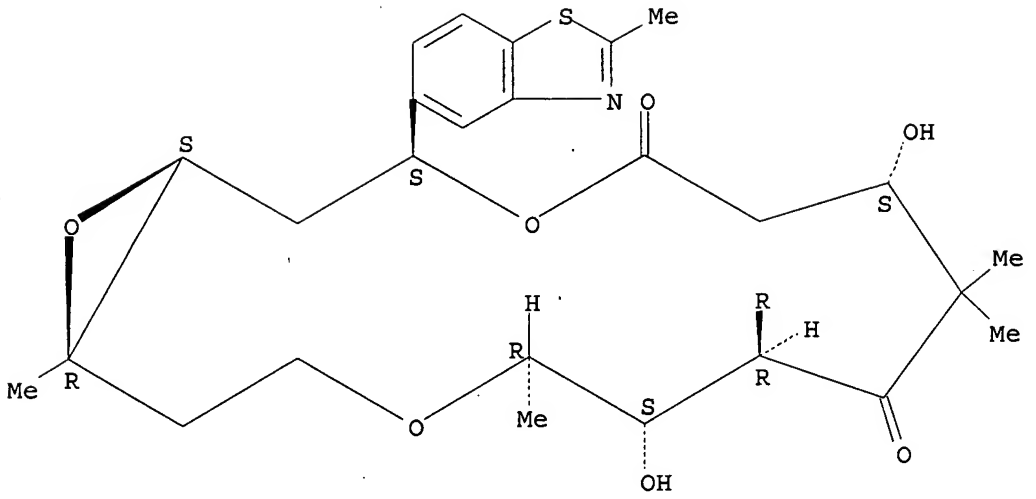
PAGE 1-B



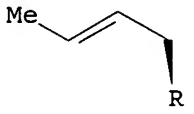
RN 369642-82-0 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 10-(2-butenyl)-7,11-dihydroxy-8,8,12,16-tetramethyl-3-(2-methyl-5-benzothiazolyl)-, (1S,3S,7S,10R,11S,12R,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



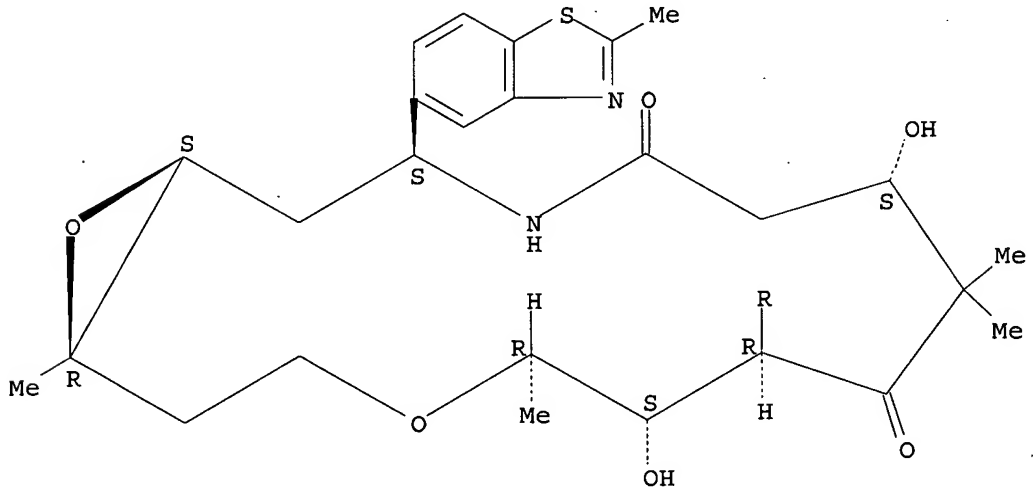
PAGE 2-A



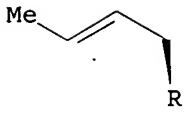
RN 369642-86-4 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 7-(2-butenyl)-6,10-dihydroxy-1,5,9,9-tetramethyl-14-(2-methyl-5-benzothiazolyl)-, (1R,5R,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



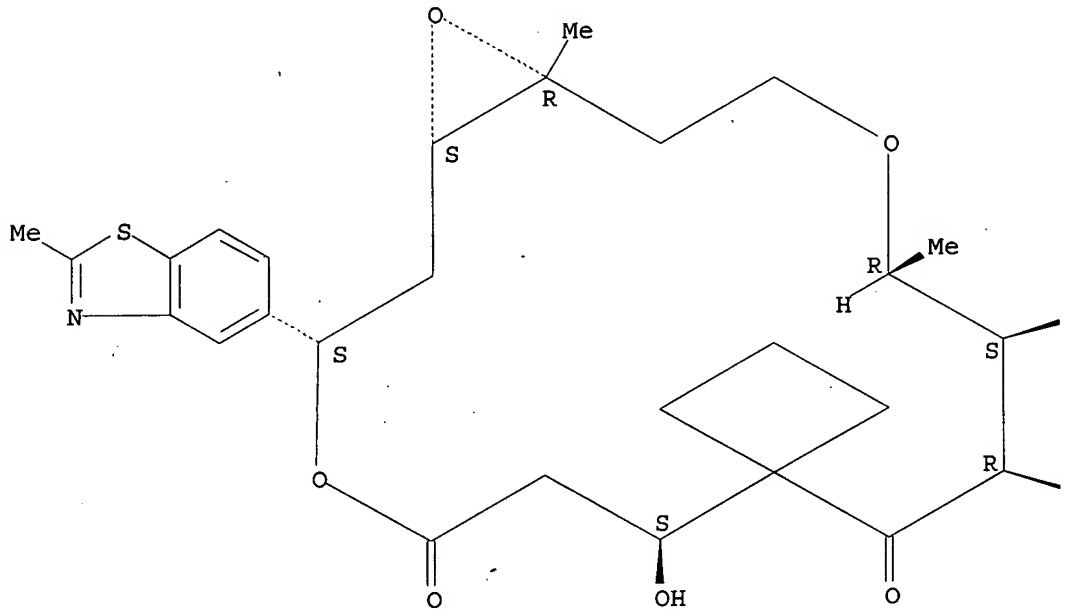
PAGE 2-A



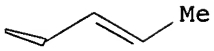
RN 369642-90-0 CAPLUS
CN Spiro[cyclobutane-1,8'-[4,13,17]trioxabicyclo[14.1.0]heptadecane]-5',9'-dione, 10'-(2-butenyl)-7',11'-dihydroxy-12',16'-dimethyl-3'-(2-methyl-5-benzothiazolyl)-, (1'S,3'S,7'S,10'R,11'S,12'R,16'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



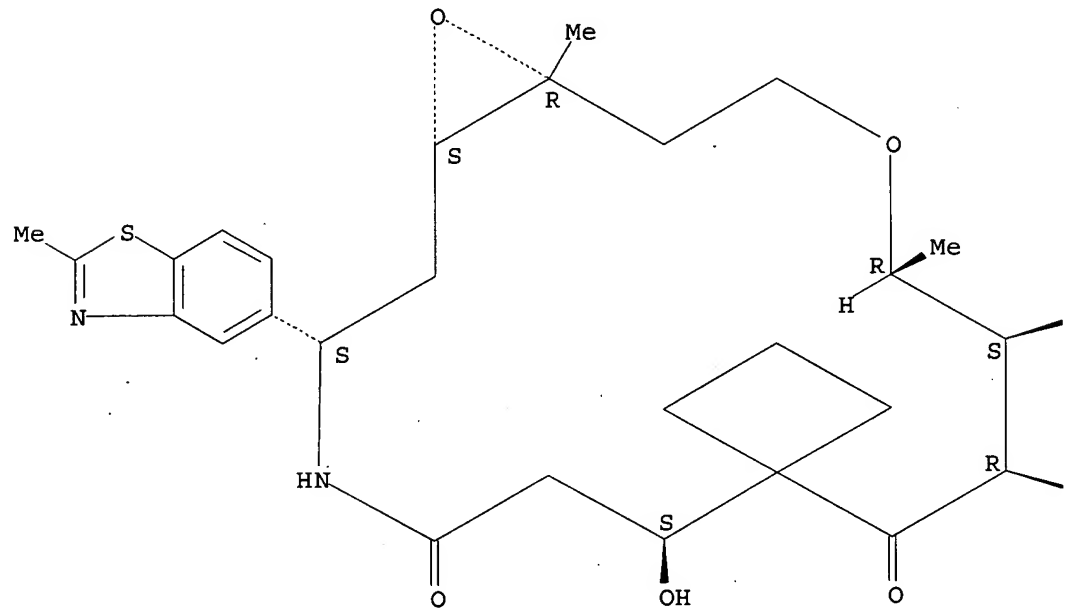
PAGE 1-B



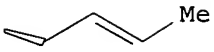
RN 369642-94-4 CAPLUS
CN Spiro[cyclobutane-1,9'-[4,17]dioxa[13]azabicyclo[14.1.0]heptadecane]-8',12'-dione, 7'-(2-butenyl)-6',10'-dihydroxy-1',5'-dimethyl-14'-(2-methyl-5-benzothiazolyl)-, (1'R,5'R,6'S,7'R,10'S,14'S,16'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



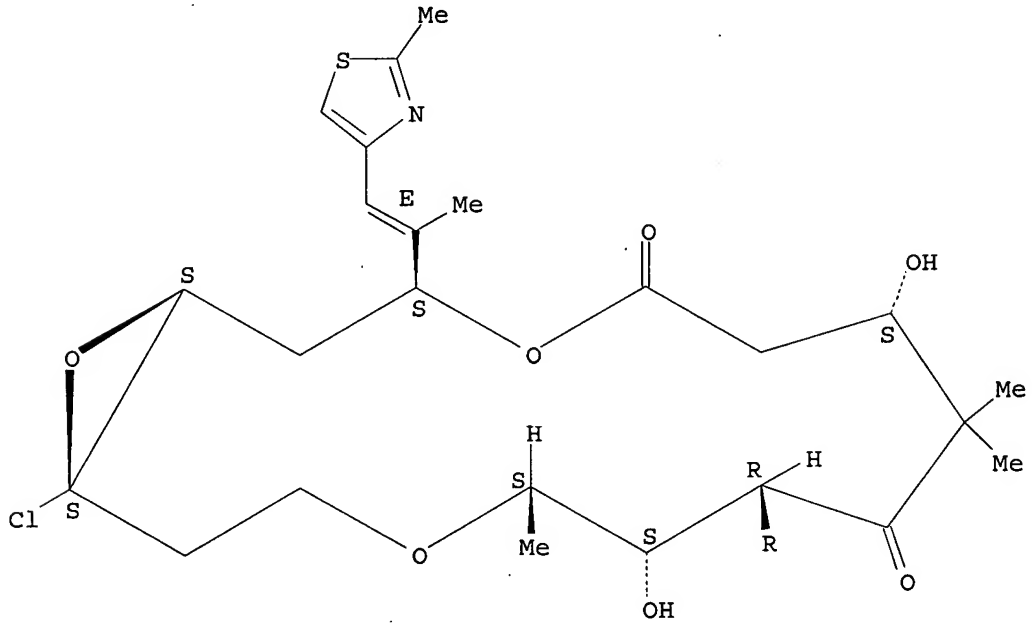
PAGE 1-B



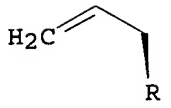
RN 369643-19-6 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 16-chloro-7,11-dihydroxy-8,8,12-trimethyl-3-[(1E)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



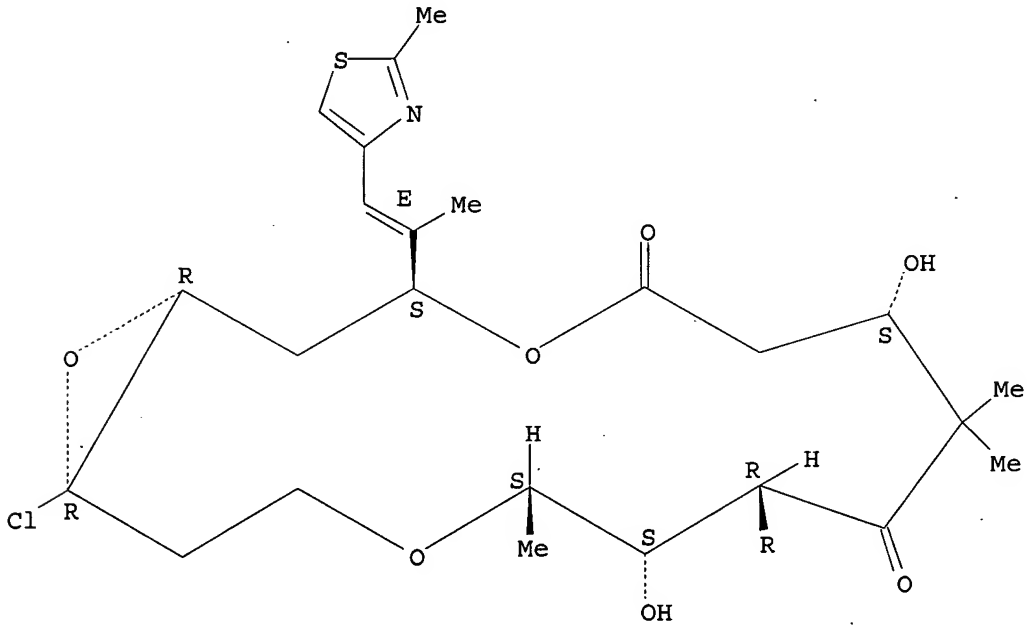
PAGE 2-A



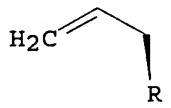
RN 369643-20-9 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 16-chloro-7,11-dihydroxy-8,8,12-trimethyl-3-[(1E)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-10-(2-propenyl)-, (1R,3S,7S,10R,11S,12S,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



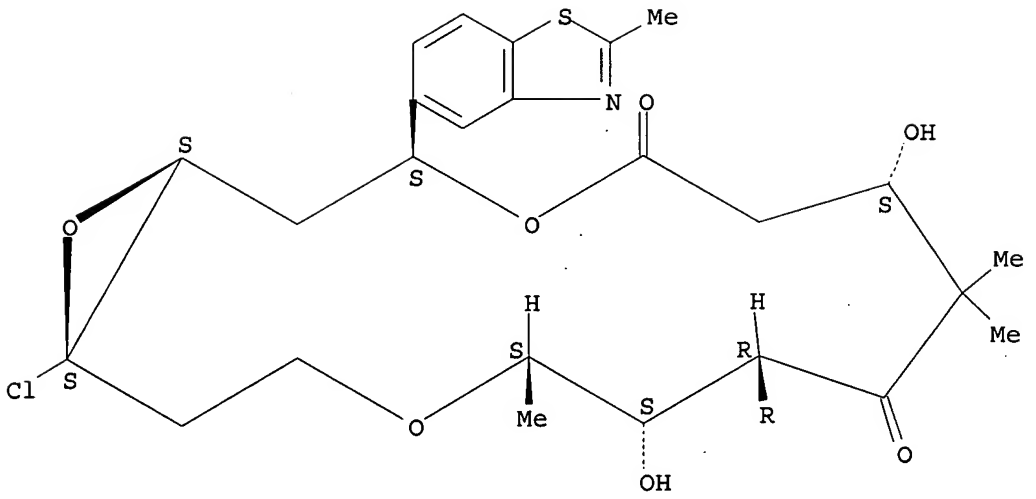
PAGE 2-A



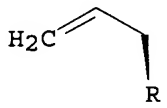
RN 369643-69-6 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 16-chloro-7,11-dihydroxy-8,8,12-trimethyl-3-(2-methyl-5-benzothiazolyl)-10-(2-propenyl)-, (1S,3S,7S,10R,11S,12S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



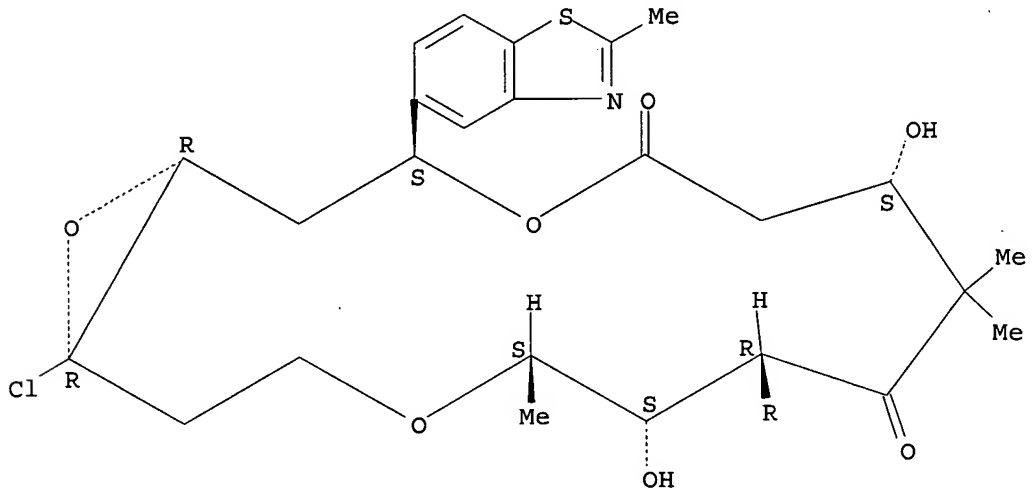
PAGE 2-A



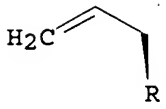
RN 369643-70-9 CAPLUS
CN 4,13,17-Trioxabicyclo[14.1.0]heptadecane-5,9-dione, 16-chloro-7,11-dihydroxy-8,8,12-trimethyl-3-(2-methyl-5-benzothiazolyl)-10-(2-propenyl)-, (1R,3S,7S,10R,11S,12S,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



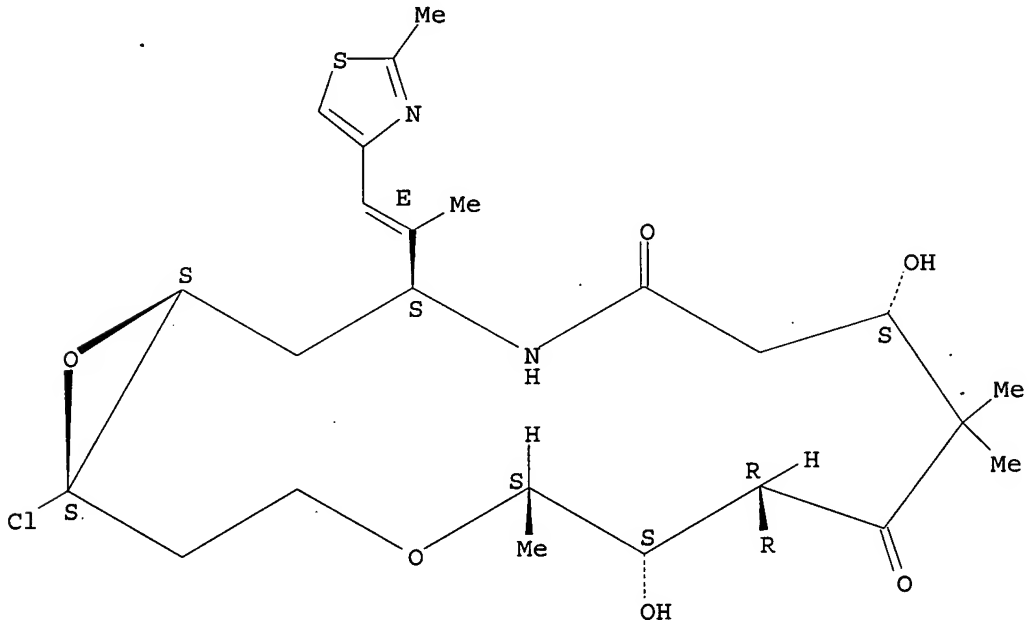
PAGE 2-A



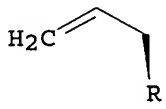
RN 369643-94-7 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 1-chloro-6,10-dihydroxy-5,9,9-trimethyl-14-[(1E)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-7-(2-propenyl)-, (1S,5S,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 2-A

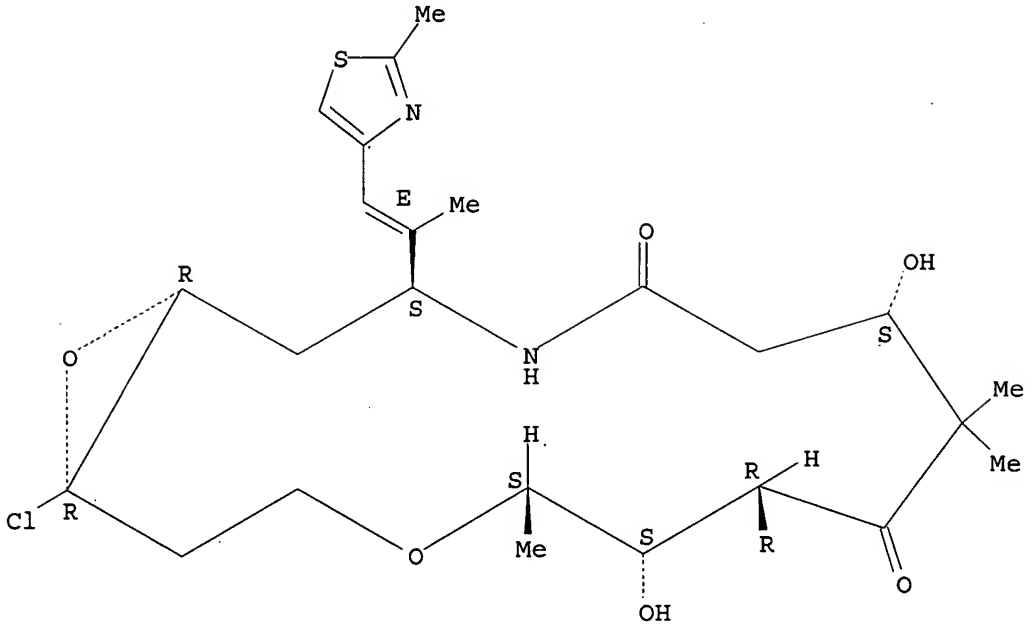


RN 369643-95-8 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 1-chloro-6,10-dihydroxy-5,9,9-trimethyl-14-[(1E)-1-methyl-2-(2-methyl-4-thiazolyl)ethenyl]-7-(2-propenyl)-, (1R,5S,6S,7R,10S,14S,16R)- (9CI) (CA INDEX NAME)

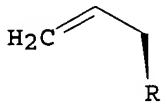
Absolute stereochemistry.

Double bond geometry as shown.

PAGE 1-A



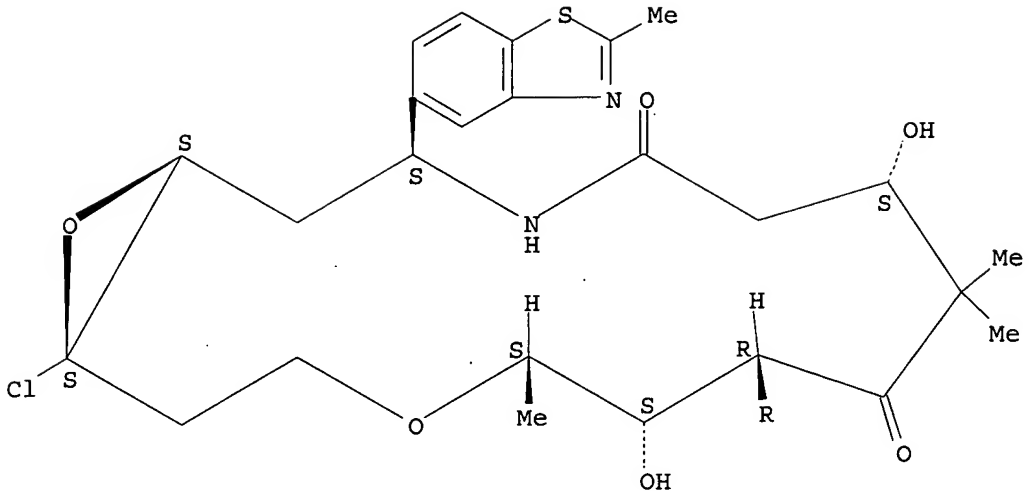
PAGE 2-A



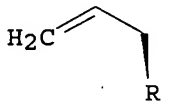
RN 369644-51-9 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 1-chloro-6,10-dihydroxy-5,9,9-trimethyl-14-(2-methyl-5-benzothiazolyl)-7-(2-propenyl)-, (1S,5S,6S,7R,10S,14S,16S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



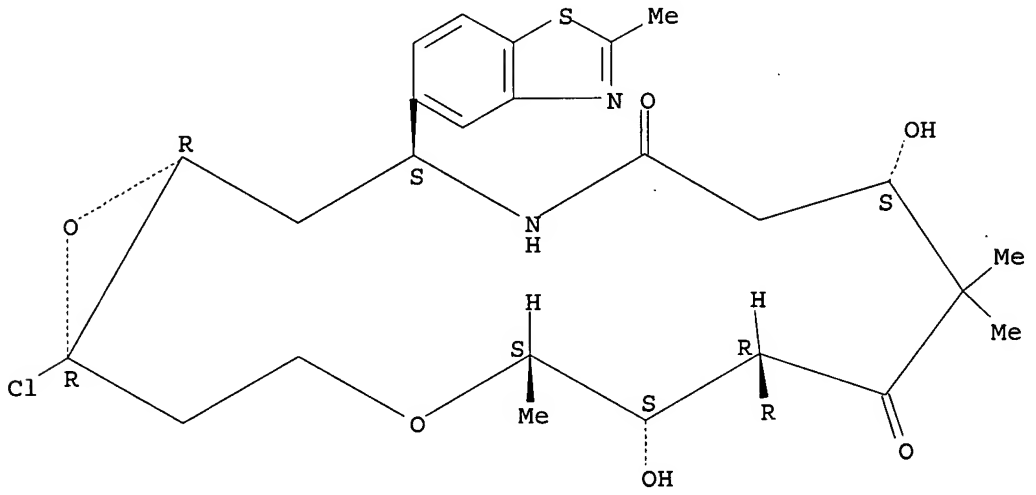
PAGE 2-A



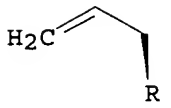
RN 369644-52-0 CAPLUS
CN 4,17-Dioxa-13-azabicyclo[14.1.0]heptadecane-8,12-dione, 1-chloro-6,10-dihydroxy-5,9,9-trimethyl-14-(2-methyl-5-benzothiazolyl)-7-(2-propenyl)-, (1R,5S,6S,7R,10S,14S,16R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



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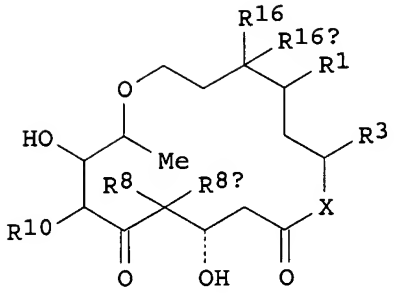

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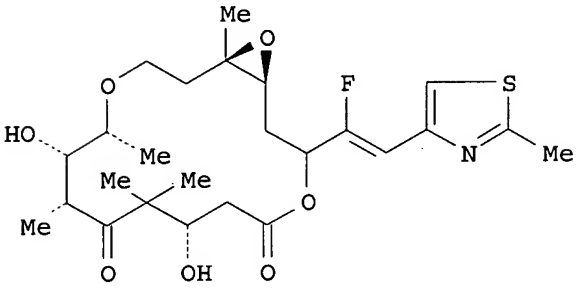

II

AB Oxa-epothilones, such as I [R3 = heteroaryl, heteroarylalkenyl, heteroarylhaloalkenyl,etc.; R8, R8a = H, alkyl, arylalkyl; R8R8a = alkylene, heteroalkene; R10 = H, alkyl, alkenyl, alkynyl; R1R16a = bond, O; R16 = H, CN, alkyl, halogen; X = O, NH], were prepared for a variety of therapeutic uses, such as treatment of malignant tumors, proliferative diseases, leukemia, and chronic inflammatory diseases, as well as for anti-angiogenic SE therapy. Thus, oxa-epothilone II was prepared via a multistep synthetic sequence starting from (R)-1,2-propanediol, and [(3S,4Z)-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-fluoro-5-(2-methyl-4-thiazolyl)-4-pentenyl]triphenylphosphonium iodide,. Pharmaceutical formulations of the prepared oxa-epothilones were discussed, but specific biol. activity data was not presented.

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.39	166.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

STN INTERNATIONAL LOGOFF AT 19:20:43 ON 21 SEP 2005